Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 09:21 PM EST

PDB ID	:	4GRG
Title	:	Crystal structure of IgE complexed with E2_79, an anti-IgE inhibitor
Authors	:	Kim, B.; Jardetzky, T.S.
Deposited on	:	2012-08-24
Resolution	:	4.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

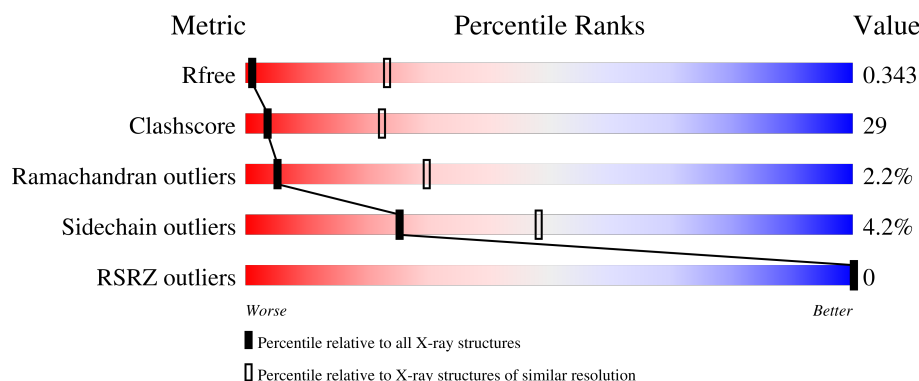|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1004 (4.62-3.86)
Clashscore	180529	1022 (4.60-3.88)
Ramachandran outliers	177936	1021 (4.66-3.82)
Sidechain outliers	177891	1006 (4.66-3.82)
RSRZ outliers	164620	1002 (4.62-3.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	41% 47% • 8%
1	B	135	41% 46% • 8%
2	C	230	62% 30% • 7%
2	D	230	62% 29% • 7%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 5154 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ANTI-IGE INHIBITOR E2_79.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			891	555	157	178	1			
1	B	124	Total	C	N	O	S	0	0	0
			891	555	157	178	1			

- Molecule 2 is a protein called Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1687	1055	311	314	7			
2	D	213	Total	C	N	O	S	0	0	0
			1685	1054	312	312	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	325	ALA	-	expression tag	UNP P01854
C	326	ASP	-	expression tag	UNP P01854
C	327	PRO	-	expression tag	UNP P01854
C	328	ALA	-	expression tag	UNP P01854
C	335	CYS	GLY	engineered mutation	UNP P01854
C	548	ALA	-	expression tag	UNP P01854
C	549	ALA	-	expression tag	UNP P01854
C	550	ASP	-	expression tag	UNP P01854
C	551	ASP	-	expression tag	UNP P01854
C	552	ASP	-	expression tag	UNP P01854
C	553	ASP	-	expression tag	UNP P01854
C	554	LYS	-	expression tag	UNP P01854
D	325	ALA	-	expression tag	UNP P01854
D	326	ASP	-	expression tag	UNP P01854
D	327	PRO	-	expression tag	UNP P01854
D	328	ALA	-	expression tag	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
D	335	CYS	GLY	engineered mutation	UNP P01854
D	548	ALA	-	expression tag	UNP P01854
D	549	ALA	-	expression tag	UNP P01854
D	550	ASP	-	expression tag	UNP P01854
D	551	ASP	-	expression tag	UNP P01854
D	552	ASP	-	expression tag	UNP P01854
D	553	ASP	-	expression tag	UNP P01854
D	554	LYS	-	expression tag	UNP P01854

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ANTI-IGE INHIBITOR E2_79

Chain A:
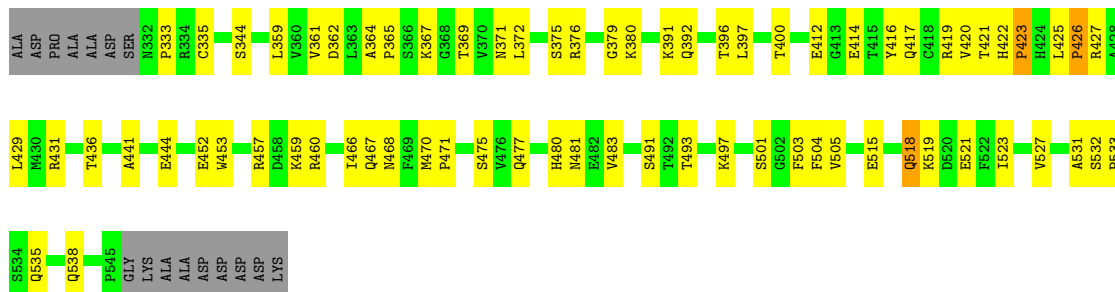
41%   47%   •   8%

• Molecule 1: ANTI-IGE INHIBITOR E2_79

Chain B:

41%   46%   •   8%

• Molecule 2: Ig epsilon chain C region

Chain C:

62%   30%   •   7%

• Molecule 2: Ig epsilon chain C region

Chain D:

62%   29%   •   7%

ALA ASP PRO ALA ALA ASP SER ASN P333 R334 S344 L359 V360 V361 D362 L363 A364 P365 S366 K367 G368 T369 V370 N371 L372 S375 R376 A377 S378 G379 K391 T396 T400 R408 E412 G413 E414 T415 Y416 R419 V420 T421 H422 P423 H424 L425 P426 L429 M430 R431

K435 T436 S437 A442 P443 E444 V445 Y446 E452 W453 R457 D458 K459 R460 T461 L462 I466 Q467 M470 P471 S475 V476 Q477 N481 E482 V483 S491 T492 T493 K497 S501 F504 V505 E515 Q518 K519 D520 E521 F522 I523 V527 A531 S532 P533

S534 Q535 Q538 P545 GLY LYS ALA ALA ASP ASP ASP LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	71.31Å 71.31Å 178.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 4.24 29.75 – 4.24	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.75-4.24) 89.3 (29.75-4.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 4.26Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC 5.5.0109	Depositor
R, R_{free}	0.270 , 0.338 0.273 , 0.343	Depositor DCC
R_{free} test set	303 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	197.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 997.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l 0.458 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5154	wwPDB-VP
Average B, all atoms (Å^2)	274.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.58	0/904	0.84	6/1235 (0.5%)
1	B	0.57	0/904	0.84	6/1235 (0.5%)
2	C	0.44	0/1731	0.58	0/2359
2	D	0.46	0/1729	0.59	0/2354
All	All	0.50	0/5268	0.68	12/7183 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	ILE	CB-CA-C	-8.96	93.67	111.60
1	B	62	ILE	CB-CA-C	-8.95	93.70	111.60
1	B	105	ASP	CB-CA-C	6.69	123.78	110.40
1	A	105	ASP	CB-CA-C	6.68	123.77	110.40
1	A	105	ASP	N-CA-C	-6.19	94.30	111.00
1	B	105	ASP	N-CA-C	-6.17	94.33	111.00
1	A	48	HIS	N-CA-C	5.80	126.67	111.00
1	B	48	HIS	N-CA-C	5.79	126.64	111.00
1	A	93	LEU	N-CA-CB	5.49	121.38	110.40
1	B	93	LEU	N-CA-CB	5.47	121.34	110.40
1	B	48	HIS	N-CA-CB	-5.36	100.95	110.60
1	A	48	HIS	N-CA-CB	-5.34	100.99	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LYS	Peptide
1	A	92	HIS	Peptide
1	B	101	LYS	Peptide
1	B	92	HIS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	891	0	829	93	0
1	B	891	0	829	99	0
2	C	1687	0	1663	85	0
2	D	1685	0	1669	69	0
All	All	5154	0	4990	290	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:TYR:CE2	2:C:412:GLU:OE1	1.81	1.31
1:A:45:TYR:HE2	2:D:412:GLU:OE1	1.27	1.17
1:A:45:TYR:CE2	2:D:412:GLU:OE1	1.99	1.16
1:A:44:ASP:OD1	1:A:48:HIS:HB2	1.50	1.10
1:B:44:ASP:OD1	1:B:48:HIS:HB2	1.50	1.10
1:B:45:TYR:CE2	2:C:412:GLU:CD	2.27	1.08
1:A:45:TYR:CE2	2:D:412:GLU:CD	2.28	1.06
2:C:422:HIS:HB3	2:C:425:LEU:HB2	1.38	1.05
1:B:45:TYR:HE2	2:C:412:GLU:OE1	1.22	1.03
1:A:62:ILE:O	1:A:62:ILE:CG2	2.07	1.02
1:B:62:ILE:CG2	1:B:62:ILE:O	2.07	1.01
1:A:67:LEU:HD13	1:A:102:HIS:CE1	1.94	1.01
1:B:67:LEU:HD13	1:B:102:HIS:CE1	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:O	1:B:62:ILE:HG22	1.64	0.94
1:B:45:TYR:CZ	2:C:412:GLU:OE2	2.19	0.94
1:A:45:TYR:CZ	2:D:412:GLU:OE2	2.20	0.94
1:A:62:ILE:O	1:A:62:ILE:HG22	1.64	0.93
1:A:89:TRP:CH2	2:D:375:SER:OG	2.21	0.92
1:B:29:GLU:O	1:B:33:LEU:HG	1.70	0.91
1:A:29:GLU:O	1:A:33:LEU:HG	1.70	0.91
1:A:89:TRP:HH2	2:D:375:SER:OG	1.54	0.89
1:A:89:TRP:HH2	2:D:375:SER:HG	0.91	0.88
1:A:90:ALA:C	1:A:92:HIS:H	1.77	0.88
2:C:429:LEU:HD21	2:D:333:PRO:HG3	1.54	0.88
1:B:89:TRP:HH2	2:C:375:SER:OG	1.57	0.88
1:B:90:ALA:C	1:B:92:HIS:H	1.77	0.88
2:C:422:HIS:CG	2:C:423:PRO:HD2	2.09	0.87
1:A:73:VAL:HG21	1:A:102:HIS:HD2	1.40	0.87
1:B:73:VAL:HG21	1:B:102:HIS:HD2	1.40	0.86
1:A:45:TYR:O	1:A:46:TRP:CD1	2.30	0.84
1:B:45:TYR:O	1:B:46:TRP:CD1	2.30	0.84
1:A:123:ASN:HB2	2:D:419:ARG:NH1	1.94	0.83
1:A:67:LEU:HD13	1:A:102:HIS:NE2	1.92	0.83
1:B:67:LEU:HD13	1:B:102:HIS:NE2	1.92	0.82
1:A:89:TRP:HH2	2:D:375:SER:CB	1.92	0.82
1:B:89:TRP:CH2	2:C:375:SER:OG	2.28	0.82
1:B:46:TRP:O	1:B:48:HIS:N	2.13	0.82
1:A:46:TRP:O	1:A:48:HIS:N	2.13	0.81
2:D:481:ASN:HD21	2:D:519:LYS:HG2	1.44	0.81
2:D:481:ASN:ND2	2:D:519:LYS:HG2	1.94	0.81
1:A:73:VAL:CG2	1:A:102:HIS:HD2	1.94	0.81
1:B:73:VAL:CG2	1:B:102:HIS:HD2	1.94	0.81
2:C:422:HIS:ND1	2:C:423:PRO:HD2	1.95	0.81
2:C:481:ASN:ND2	2:C:519:LYS:HG2	1.96	0.80
1:B:45:TYR:CZ	2:C:412:GLU:CD	2.55	0.80
2:D:422:HIS:CD2	2:D:423:PRO:HD2	2.17	0.79
2:C:425:LEU:HD12	2:C:426:PRO:HD2	1.64	0.79
2:C:481:ASN:HD21	2:C:519:LYS:HG2	1.46	0.79
1:A:60:LEU:HD13	1:A:95:ILE:HG12	1.65	0.78
1:B:60:LEU:HD13	1:B:95:ILE:HG12	1.65	0.78
1:A:44:ASP:C	1:A:46:TRP:H	1.86	0.78
1:B:44:ASP:C	1:B:46:TRP:H	1.86	0.78
1:B:89:TRP:HH2	2:C:375:SER:HG	0.86	0.77
1:B:123:ASN:HB2	2:C:419:ARG:NH1	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:TYR:O	1:B:46:TRP:HD1	1.70	0.75
2:C:371:ASN:HB2	2:C:421:THR:HB	1.68	0.75
2:D:371:ASN:HB2	2:D:421:THR:HB	1.67	0.75
1:A:45:TYR:O	1:A:46:TRP:HD1	1.71	0.74
1:B:81:ARG:HH12	2:C:379:GLY:HA3	1.52	0.74
1:A:120:SER:HA	1:A:128:LEU:HD23	1.70	0.73
1:B:120:SER:HA	1:B:128:LEU:HD23	1.70	0.73
2:C:431:ARG:HH22	2:D:333:PRO:HD3	1.52	0.73
1:A:73:VAL:CG2	1:A:102:HIS:CD2	2.73	0.72
1:A:81:ARG:HH12	2:D:379:GLY:HA3	1.54	0.72
1:B:73:VAL:CG2	1:B:102:HIS:CD2	2.73	0.72
1:B:81:ARG:HH22	2:C:379:GLY:HA3	1.55	0.70
1:A:45:TYR:OH	2:D:412:GLU:OE2	2.08	0.70
1:A:84:LEU:HD23	1:A:105:ASP:O	1.92	0.69
1:B:84:LEU:HD23	1:B:105:ASP:O	1.92	0.69
1:B:89:TRP:HH2	2:C:375:SER:CB	2.06	0.69
1:A:52:HIS:HB3	1:A:86:LEU:HD22	1.75	0.68
1:B:52:HIS:HB3	1:B:86:LEU:HD22	1.75	0.68
1:B:52:HIS:CD2	1:B:86:LEU:HD13	2.29	0.67
1:A:52:HIS:CD2	1:A:86:LEU:HD13	2.29	0.67
1:B:21:ALA:HA	1:B:24:ALA:HB3	1.77	0.67
1:A:21:ALA:HA	1:A:24:ALA:HB3	1.77	0.67
1:A:73:VAL:HG11	1:A:103:GLY:O	1.95	0.66
1:B:73:VAL:HG11	1:B:103:GLY:O	1.95	0.66
1:B:67:LEU:CD1	1:B:102:HIS:CE1	2.76	0.66
1:A:67:LEU:CD1	1:A:102:HIS:CE1	2.76	0.65
2:C:441:ALA:HB3	2:C:470:MET:HG2	1.79	0.65
1:A:73:VAL:HG22	1:A:102:HIS:CD2	2.32	0.65
1:A:81:ARG:HH22	2:D:379:GLY:HA3	1.62	0.65
1:A:89:TRP:HH2	2:D:375:SER:HB2	1.62	0.65
1:A:45:TYR:CZ	2:D:412:GLU:CD	2.66	0.64
1:A:117:PHE:CD1	1:A:132:LEU:HB3	2.33	0.64
1:B:73:VAL:HG22	1:B:102:HIS:CD2	2.32	0.64
2:D:422:HIS:HB3	2:D:425:LEU:HG	1.79	0.64
1:B:117:PHE:CD1	1:B:132:LEU:HB3	2.33	0.64
1:B:117:PHE:HA	1:B:132:LEU:HD13	1.77	0.64
1:A:74:ASN:HD21	1:A:104:ALA:HA	1.63	0.64
1:A:117:PHE:HA	1:A:132:LEU:HD13	1.77	0.64
2:C:521:GLU:OE1	2:C:521:GLU:HA	1.97	0.64
1:A:90:ALA:C	1:A:92:HIS:N	2.50	0.64
1:B:74:ASN:HD21	1:B:104:ALA:HA	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ALA:C	1:B:92:HIS:N	2.50	0.64
2:C:431:ARG:NH2	2:D:333:PRO:HD3	2.12	0.64
1:B:90:ALA:O	1:B:92:HIS:N	2.32	0.63
1:A:90:ALA:O	1:A:92:HIS:N	2.32	0.63
2:D:420:VAL:HB	2:D:429:LEU:HB2	1.81	0.63
1:A:44:ASP:C	1:A:46:TRP:N	2.52	0.63
1:B:44:ASP:C	1:B:46:TRP:N	2.52	0.63
1:A:44:ASP:O	1:A:46:TRP:N	2.30	0.63
1:B:44:ASP:O	1:B:46:TRP:N	2.31	0.63
1:B:81:ARG:HH12	2:C:379:GLY:CA	2.11	0.63
1:A:46:TRP:HB3	1:A:48:HIS:CE1	2.33	0.63
1:A:62:ILE:O	1:A:62:ILE:HG23	1.96	0.62
1:B:46:TRP:HB3	1:B:48:HIS:CE1	2.34	0.62
2:D:435:LYS:O	2:D:435:LYS:HG3	1.98	0.62
1:B:62:ILE:O	1:B:62:ILE:HG23	1.96	0.62
1:B:45:TYR:OH	2:C:412:GLU:OE2	2.17	0.62
1:B:73:VAL:HG12	1:B:104:ALA:HA	1.80	0.62
1:A:73:VAL:HG12	1:A:104:ALA:HA	1.80	0.62
2:D:521:GLU:HA	2:D:521:GLU:OE1	1.98	0.62
1:B:44:ASP:OD1	1:B:48:HIS:CB	2.40	0.61
1:A:44:ASP:OD1	1:A:48:HIS:CB	2.40	0.61
1:A:73:VAL:HG12	1:A:73:VAL:O	2.02	0.60
1:B:73:VAL:HG12	1:B:73:VAL:O	2.02	0.60
2:C:362:ASP:HA	2:C:396:THR:HG23	1.84	0.59
2:D:372:LEU:CD2	2:D:420:VAL:HG22	2.34	0.58
2:C:372:LEU:CD2	2:C:420:VAL:HG22	2.34	0.58
2:C:420:VAL:HB	2:C:429:LEU:HB2	1.86	0.58
1:B:56:MET:HG3	1:B:57:LEU:HD12	1.86	0.58
1:A:56:MET:HG3	1:A:57:LEU:HD12	1.86	0.57
2:C:333:PRO:HD3	2:D:431:ARG:NH2	2.19	0.57
1:B:81:ARG:NH1	2:C:379:GLY:HA3	2.19	0.57
2:C:376:ARG:HD2	2:C:414:GLU:OE2	2.04	0.57
2:C:444:GLU:HG2	2:D:453:TRP:CE2	2.39	0.57
1:B:81:ARG:NH2	2:C:379:GLY:HA3	2.21	0.56
2:C:453:TRP:CE2	2:D:444:GLU:HG2	2.40	0.56
1:A:73:VAL:HG21	1:A:102:HIS:CD2	2.31	0.56
1:B:93:LEU:HD11	2:C:427:ARG:NH2	2.20	0.56
2:C:364:ALA:HB3	2:C:367:LYS:HG3	1.88	0.56
1:B:73:VAL:HG21	1:B:102:HIS:CD2	2.31	0.55
1:A:40:VAL:HG22	1:A:71:ALA:HB2	1.87	0.55
2:C:422:HIS:CE1	2:C:423:PRO:HD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:475:SER:HB2	2:C:527:VAL:HB	1.89	0.55
2:D:334:ARG:HH12	2:D:364:ALA:HB2	1.72	0.55
1:B:40:VAL:HG22	1:B:71:ALA:HB2	1.87	0.55
2:C:365:PRO:HB3	2:C:391:LYS:HE2	1.88	0.55
2:D:475:SER:HB2	2:D:527:VAL:HB	1.89	0.55
2:C:444:GLU:O	2:C:466:ILE:HA	2.06	0.55
1:B:123:ASN:CB	2:C:419:ARG:NH1	2.70	0.54
1:B:34:THR:HA	1:B:38:ALA:H	1.72	0.54
1:A:81:ARG:HH12	2:D:379:GLY:CA	2.19	0.54
1:A:34:THR:HA	1:A:38:ALA:H	1.72	0.54
2:C:425:LEU:CD1	2:C:426:PRO:HD2	2.35	0.54
1:A:56:MET:HE2	1:A:86:LEU:HD23	1.90	0.54
2:D:376:ARG:HD2	2:D:414:GLU:OE2	2.08	0.53
1:A:79:THR:O	1:A:81:ARG:HG2	2.09	0.53
1:B:79:THR:O	1:B:81:ARG:HG2	2.09	0.53
1:A:81:ARG:NH1	2:D:379:GLY:HA3	2.24	0.53
1:B:19:LEU:HD12	1:B:20:GLU:N	2.24	0.53
1:A:99:LEU:O	1:A:102:HIS:O	2.26	0.53
1:B:56:MET:HE1	1:B:86:LEU:HD23	1.91	0.53
1:B:99:LEU:O	1:B:102:HIS:O	2.26	0.53
1:A:19:LEU:HD12	1:A:20:GLU:N	2.24	0.53
1:A:40:VAL:CG2	1:A:71:ALA:HB2	2.39	0.53
2:D:364:ALA:HB3	2:D:367:LYS:HG3	1.91	0.53
1:B:40:VAL:CG2	1:B:71:ALA:HB2	2.39	0.53
1:A:84:LEU:CD2	1:A:105:ASP:O	2.57	0.52
1:B:84:LEU:CD2	1:B:105:ASP:O	2.57	0.52
2:C:441:ALA:HB3	2:C:470:MET:CG	2.39	0.52
2:C:392:GLN:HB2	2:C:396:THR:HB	1.91	0.52
1:A:20:GLU:HA	1:A:23:ARG:HH22	1.74	0.52
1:B:20:GLU:HA	1:B:23:ARG:HH22	1.74	0.52
1:A:56:MET:CE	1:A:86:LEU:HD23	2.40	0.52
1:B:56:MET:CE	1:B:86:LEU:HD23	2.40	0.52
2:D:444:GLU:O	2:D:466:ILE:HA	2.10	0.51
1:B:19:LEU:O	1:B:22:ALA:HB3	2.10	0.51
1:B:59:HIS:HA	1:B:61:GLU:OE1	2.11	0.51
1:A:19:LEU:O	1:A:22:ALA:HB3	2.10	0.51
1:A:59:HIS:HA	1:A:61:GLU:OE1	2.11	0.51
2:C:422:HIS:HB3	2:C:425:LEU:CB	2.26	0.51
1:A:52:HIS:HD2	1:A:86:LEU:CD1	2.23	0.51
1:B:52:HIS:HD2	1:B:86:LEU:CD1	2.23	0.51
2:C:493:THR:HG21	2:D:493:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:481:ASN:HD21	2:D:519:LYS:CG	2.21	0.50
2:C:361:VAL:HG12	2:C:362:ASP:N	2.26	0.50
1:B:46:TRP:O	1:B:48:HIS:CG	2.65	0.50
1:A:46:TRP:O	1:A:48:HIS:CG	2.64	0.50
2:C:372:LEU:HD22	2:C:420:VAL:HG22	1.93	0.50
2:D:365:PRO:HB3	2:D:391:LYS:HE2	1.93	0.50
2:C:359:LEU:HD13	2:C:400:THR:HG22	1.94	0.50
1:B:123:ASN:HB2	2:C:419:ARG:HH12	1.75	0.49
1:A:29:GLU:O	1:A:32:ILE:N	2.46	0.49
1:A:52:HIS:CD2	1:A:86:LEU:CD1	2.95	0.49
2:D:359:LEU:HD13	2:D:400:THR:HG22	1.94	0.49
1:B:29:GLU:O	1:B:32:ILE:N	2.46	0.49
2:C:396:THR:HG22	2:C:397:LEU:N	2.27	0.49
2:C:481:ASN:HD21	2:C:519:LYS:CG	2.22	0.49
1:B:52:HIS:CD2	1:B:86:LEU:CD1	2.95	0.49
1:A:81:ARG:HA	1:A:85:HIS:ND1	2.28	0.48
2:D:372:LEU:HD22	2:D:420:VAL:HG22	1.95	0.48
1:A:81:ARG:HH12	2:D:378:SER:C	2.16	0.48
1:B:93:LEU:HD11	2:C:427:ARG:HH22	1.79	0.48
1:B:81:ARG:HA	1:B:85:HIS:ND1	2.28	0.48
1:A:15:GLY:O	1:A:18:LEU:HB3	2.14	0.48
1:B:15:GLY:O	1:B:18:LEU:HB3	2.14	0.48
2:D:361:VAL:HG12	2:D:362:ASP:N	2.28	0.48
1:B:123:ASN:CA	2:C:419:ARG:CZ	2.92	0.48
2:C:452:GLU:HB2	2:C:460:ARG:NH2	2.29	0.48
2:C:452:GLU:CD	2:C:457:ARG:HB2	2.34	0.48
2:C:519:LYS:NZ	2:C:521:GLU:HB2	2.28	0.48
2:D:422:HIS:HB3	2:D:425:LEU:CG	2.42	0.47
2:D:467:GLN:HA	2:D:504:PHE:HA	1.96	0.47
1:B:123:ASN:HA	2:C:419:ARG:CZ	2.44	0.47
1:A:95:ILE:O	1:A:98:VAL:HG12	2.15	0.47
1:B:95:ILE:O	1:B:98:VAL:HG12	2.15	0.47
2:C:422:HIS:CG	2:C:423:PRO:CD	2.92	0.47
2:D:334:ARG:NE	2:D:362:ASP:O	2.48	0.46
2:C:519:LYS:HZ3	2:C:521:GLU:HB2	1.78	0.46
1:A:121:ILE:C	1:A:124:GLY:H	2.19	0.46
1:B:89:TRP:HH2	2:C:375:SER:HB2	1.80	0.46
1:B:121:ILE:C	1:B:124:GLY:H	2.19	0.46
2:D:459:LYS:O	2:D:460:ARG:HD3	2.14	0.46
1:B:114:LYS:HA	1:B:118:ASP:OD2	2.16	0.46
2:D:452:GLU:HB2	2:D:460:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:NH2	2:D:379:GLY:HA3	2.29	0.46
1:B:45:TYR:CZ	2:C:412:GLU:OE1	2.53	0.46
1:A:45:TYR:OH	2:D:408:ARG:NE	2.48	0.46
1:A:114:LYS:HA	1:A:118:ASP:OD2	2.16	0.46
1:B:54:ALA:O	1:B:57:LEU:O	2.33	0.46
1:A:54:ALA:O	1:A:57:LEU:O	2.33	0.45
2:C:523:ILE:CG2	2:C:538:GLN:HB2	2.47	0.45
2:D:422:HIS:CG	2:D:423:PRO:HD2	2.51	0.45
2:C:467:GLN:HA	2:C:504:PHE:HA	1.99	0.45
2:C:470:MET:HA	2:C:471:PRO:C	2.36	0.45
1:A:81:ARG:NH1	2:D:378:SER:O	2.50	0.45
1:A:123:ASN:CB	2:D:419:ARG:NH1	2.74	0.45
1:B:73:VAL:O	1:B:73:VAL:CG1	2.65	0.45
1:A:73:VAL:O	1:A:73:VAL:CG1	2.65	0.44
1:B:77:GLY:O	1:B:80:GLY:N	2.48	0.44
2:D:519:LYS:NZ	2:D:521:GLU:HB2	2.32	0.44
1:A:77:GLY:O	1:A:80:GLY:N	2.48	0.44
1:B:20:GLU:HA	1:B:23:ARG:NH2	2.31	0.44
1:A:20:GLU:HA	1:A:23:ARG:NH2	2.32	0.44
1:A:23:ARG:HB3	1:A:23:ARG:CZ	2.48	0.44
2:D:362:ASP:HA	2:D:396:THR:HB	2.00	0.44
1:B:23:ARG:HB3	1:B:23:ARG:CZ	2.48	0.44
1:B:52:HIS:HD2	1:B:86:LEU:HD13	1.80	0.44
1:A:52:HIS:HD2	1:A:86:LEU:HD13	1.80	0.44
2:C:459:LYS:O	2:C:460:ARG:HD3	2.17	0.43
2:D:515:GLU:O	2:D:518:GLN:HG3	2.17	0.43
2:C:429:LEU:CD2	2:D:333:PRO:HG3	2.36	0.43
2:C:480:HIS:HD2	2:C:521:GLU:O	2.01	0.43
2:C:361:VAL:CG1	2:C:362:ASP:N	2.81	0.43
2:D:523:ILE:CG2	2:D:538:GLN:HB2	2.48	0.43
2:C:359:LEU:CD1	2:C:400:THR:HG22	2.49	0.43
1:B:58:GLY:HA2	1:B:95:ILE:HD11	2.01	0.43
1:B:59:HIS:C	1:B:61:GLU:N	2.72	0.43
1:A:58:GLY:HA2	1:A:95:ILE:HD11	2.01	0.43
1:A:110:ASP:OD1	1:A:114:LYS:N	2.49	0.43
2:C:441:ALA:CB	2:C:470:MET:HG2	2.47	0.43
2:C:376:ARG:NH2	2:C:380:LYS:HB3	2.34	0.43
2:C:376:ARG:HD3	2:C:416:TYR:CE2	2.54	0.42
2:C:467:GLN:O	2:C:468:ASN:HB2	2.19	0.42
2:D:442:ALA:HA	2:D:443:PRO:HD3	1.85	0.42
1:A:59:HIS:C	1:A:61:GLU:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:453:TRP:HB2	2:D:446:TYR:OH	2.19	0.42
1:A:42:ALA:O	1:A:49:THR:HA	2.19	0.42
1:B:110:ASP:OD1	1:B:114:LYS:N	2.50	0.42
2:D:452:GLU:CD	2:D:457:ARG:HB2	2.39	0.42
1:B:42:ALA:O	1:B:49:THR:HA	2.20	0.42
1:A:56:MET:HG3	1:A:57:LEU:H	1.84	0.42
1:B:56:MET:HG3	1:B:57:LEU:H	1.84	0.42
2:D:462:LEU:N	2:D:462:LEU:HD23	2.35	0.42
2:D:422:HIS:O	2:D:425:LEU:HB2	2.20	0.41
2:D:531:ALA:O	2:D:535:GLN:HA	2.20	0.41
2:C:515:GLU:O	2:C:518:GLN:HG3	2.19	0.41
2:D:361:VAL:CG1	2:D:362:ASP:N	2.83	0.41
2:D:376:ARG:HD3	2:D:416:TYR:CE2	2.56	0.41
2:C:531:ALA:O	2:C:535:GLN:HA	2.20	0.41
1:B:81:ARG:HH12	2:C:379:GLY:N	2.19	0.41
2:C:417:GLN:HG3	2:C:431:ARG:O	2.21	0.41
2:C:470:MET:HA	2:C:471:PRO:O	2.20	0.41
2:D:470:MET:HA	2:D:471:PRO:C	2.40	0.41
2:D:532:SER:HA	2:D:533:PRO:HA	1.70	0.41
2:C:468:ASN:N	2:C:503:PHE:O	2.51	0.41
2:C:480:HIS:O	2:C:481:ASN:HB2	2.21	0.41
1:A:45:TYR:O	1:A:45:TYR:CG	2.74	0.40
1:B:45:TYR:O	1:B:45:TYR:CG	2.74	0.40
1:A:19:LEU:O	1:A:20:GLU:C	2.59	0.40
2:C:532:SER:HA	2:C:533:PRO:HA	1.71	0.40
1:A:25:GLY:HA2	1:A:62:ILE:HD12	2.03	0.40
1:B:19:LEU:O	1:B:20:GLU:C	2.59	0.40
1:B:25:GLY:HA2	1:B:62:ILE:HD12	2.03	0.40
1:B:59:HIS:C	1:B:61:GLU:H	2.24	0.40
2:D:436:THR:HG23	2:D:471:PRO:HG3	2.04	0.40
1:B:93:LEU:CD1	2:C:427:ARG:HH22	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/135 (90%)	94 (77%)	22 (18%)	6 (5%)	2	17
1	B	122/135 (90%)	95 (78%)	21 (17%)	6 (5%)	2	17
2	C	212/230 (92%)	199 (94%)	11 (5%)	2 (1%)	14	50
2	D	211/230 (92%)	202 (96%)	8 (4%)	1 (0%)	25	63
All	All	667/730 (91%)	590 (88%)	62 (9%)	15 (2%)	5	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	GLY
1	B	47	GLY
2	C	423	PRO
2	D	426	PRO
2	C	426	PRO
1	A	45	TYR
1	A	91	ASP
1	B	45	TYR
1	B	91	ASP
1	A	125	ASN
1	B	125	ASN
1	A	50	PRO
1	A	65	VAL
1	B	50	PRO
1	B	65	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/105 (80%)	84 (100%)	0	100	100
1	B	84/105 (80%)	84 (100%)	0	100	100
2	C	189/200 (94%)	178 (94%)	11 (6%)	17	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	189/200 (94%)	177 (94%)	12 (6%)	15	37
All	All	546/610 (90%)	523 (96%)	23 (4%)	25	48

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	335	CYS
2	C	344	SER
2	C	369	THR
2	C	436	THR
2	C	477	GLN
2	C	483	VAL
2	C	491	SER
2	C	497	LYS
2	C	501	SER
2	C	505	VAL
2	C	518	GLN
2	D	334	ARG
2	D	344	SER
2	D	369	THR
2	D	425	LEU
2	D	437	SER
2	D	477	GLN
2	D	483	VAL
2	D	491	SER
2	D	497	LYS
2	D	501	SER
2	D	505	VAL
2	D	518	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	48	HIS
1	A	102	HIS
1	A	109	GLN
1	B	43	ASN
1	B	48	HIS
1	B	102	HIS
1	B	109	GLN

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Mol	Chain	Res	Type
2	C	417	GLN
2	C	481	ASN
2	D	392	GLN
2	D	417	GLN
2	D	422	HIS
2	D	424	HIS
2	D	481	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	124/135 (91%)	-0.90	0	100	100	166, 261, 405, 498	0
1	B	124/135 (91%)	-0.87	0	100	100	164, 273, 402, 596	0
2	C	214/230 (93%)	-0.98	0	100	100	132, 263, 401, 798	0
2	D	213/230 (92%)	-0.96	0	100	100	142, 258, 400, 783	0
All	All	675/730 (92%)	-0.94	0	100	100	132, 263, 404, 798	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.