



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2024 – 01:19 pm BST

PDB ID : 8S5F
Title : Crystal structure of the HExxH domain of ChlBHExxH a novel alpha-ketoglutarate dependent oxygenase
Authors : de la Mora, E.; Amara, P.; Usclat, A.; Morishita, Y.; Morinaka, B.; Nicolet, Y.
Deposited on : 2024-02-23
Resolution : 2.80 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
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

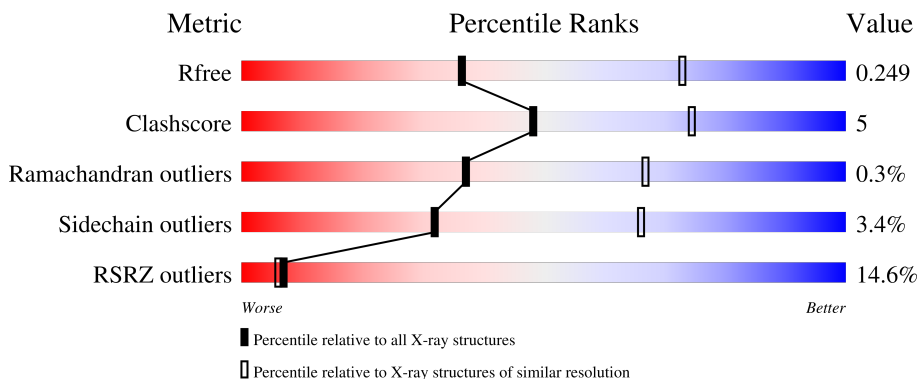
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


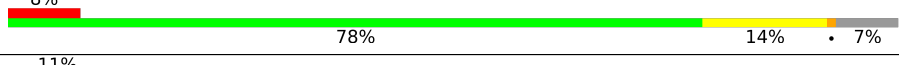

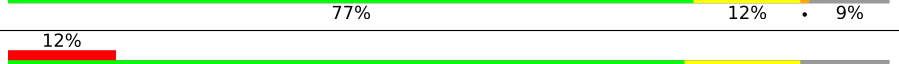

The reported resolution of this entry is 2.80 Å.

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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 $\leq 5\%$. 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	368	
1	B	368	
1	C	368	
1	D	368	
1	E	368	

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Mol	Chain	Length	Quality of chain
1	F	368	 <p>A horizontal bar chart showing the quality distribution of chain F. The bar is divided into four segments: a red segment representing 21%, a green segment representing 76%, a yellow segment representing 10%, and a grey segment representing 13%.</p>

2 Entry composition [i](#)

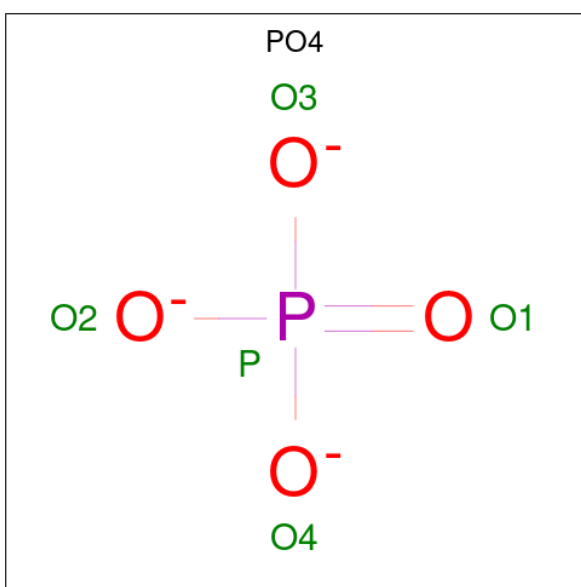
There are 2 unique types of molecules in this entry. The entry contains 16156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ChlH from Chlorogloeopsis sp..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	Total 2747	C 1753	N 475	O 513	S 6	0	3	0
1	B	342	Total 2741	C 1749	N 474	O 512	S 6	0	1	0
1	C	342	Total 2735	C 1746	N 473	O 510	S 6	0	0	0
1	D	335	Total 2682	C 1715	N 465	O 496	S 6	0	0	0
1	E	331	Total 2650	C 1700	N 452	O 493	S 5	0	0	0
1	F	320	Total 2571	C 1648	N 440	O 478	S 5	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

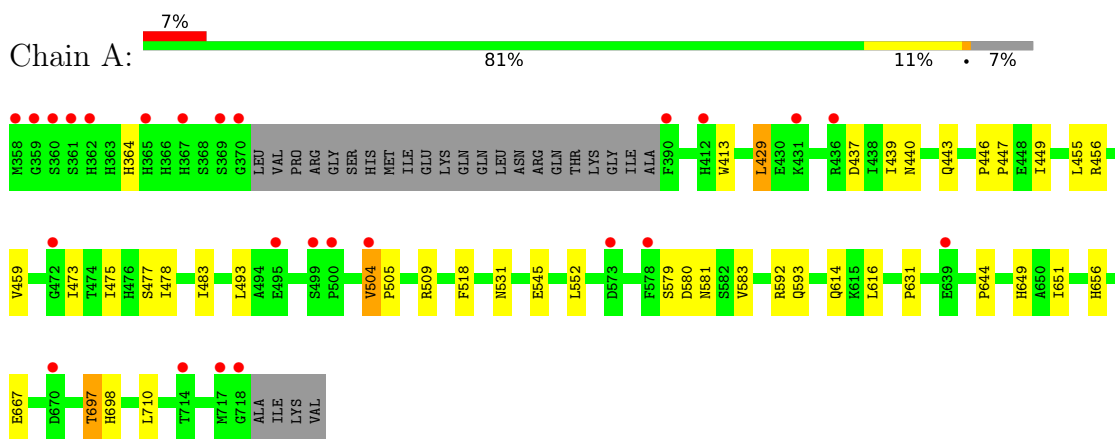


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

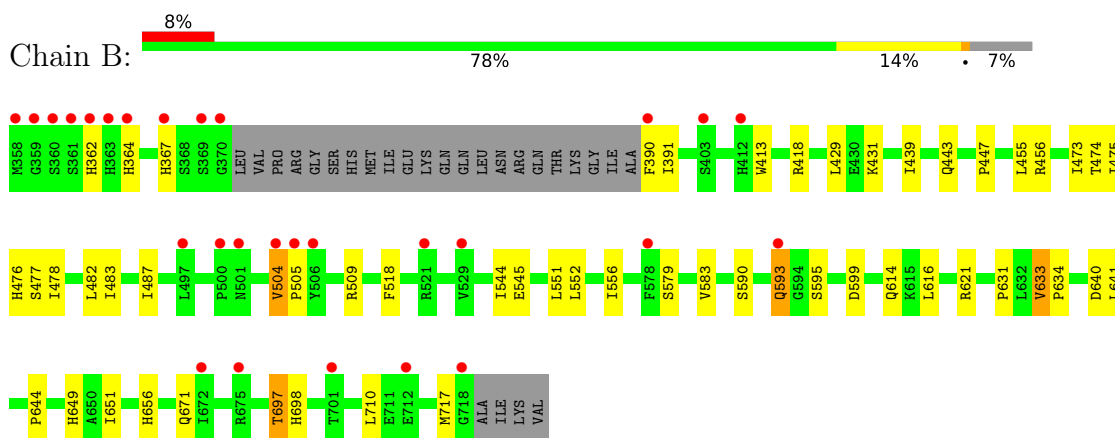
3 Residue-property plots [i](#)

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.

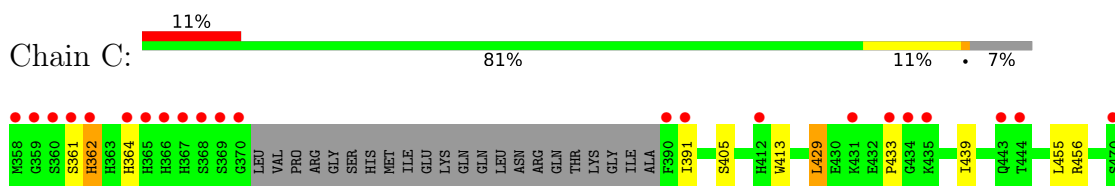
- Molecule 1: ChlH from Chlorogloeopsis sp.

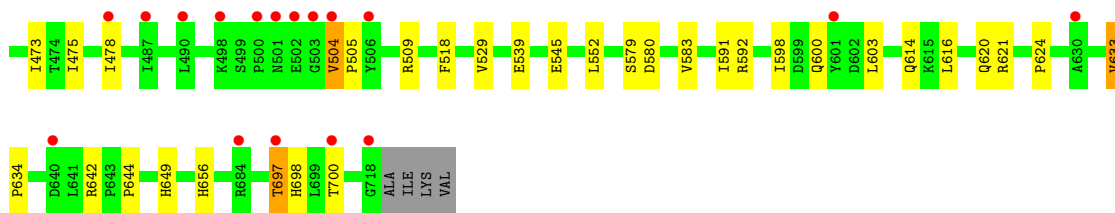


- Molecule 1: ChlH from Chlorogloeopsis sp.

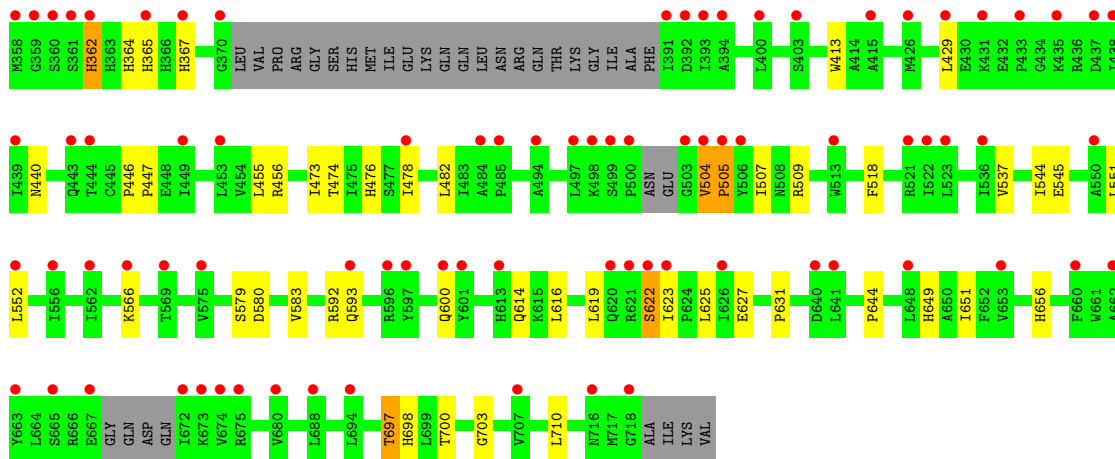
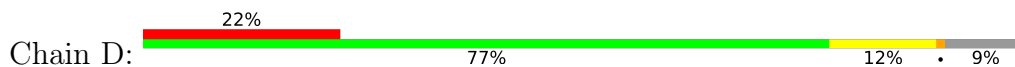


- Molecule 1: ChlH from Chlorogloeopsis sp.

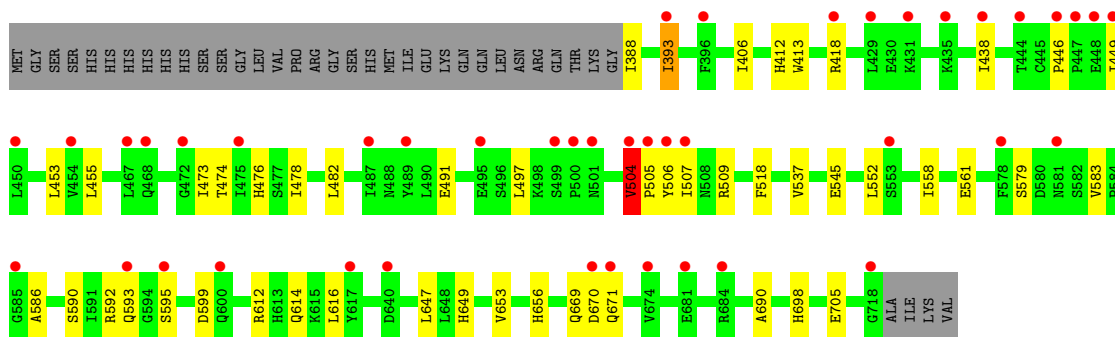
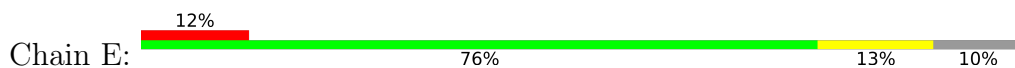




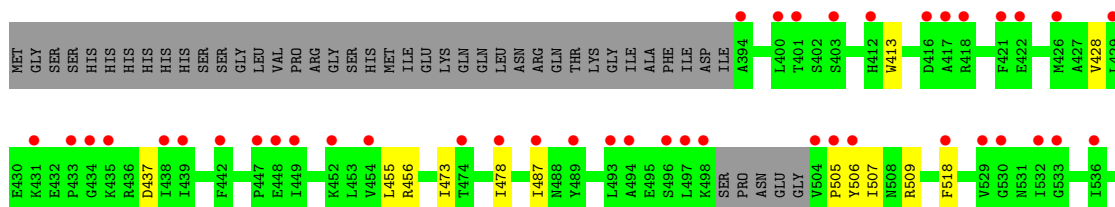
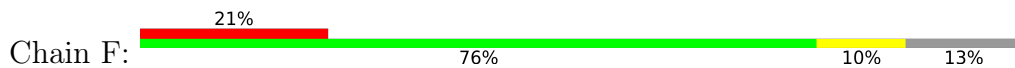
● Molecule 1: ChlH from Chlorogloeopsis sp.

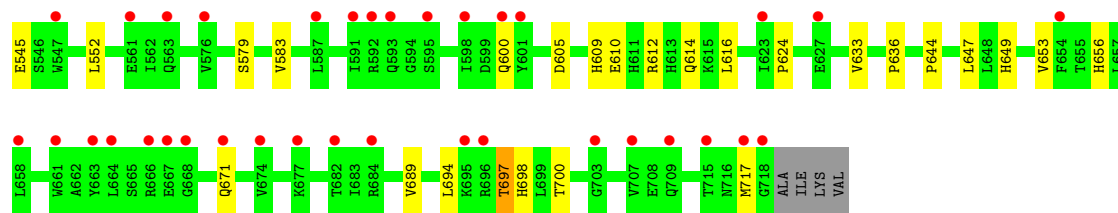


● Molecule 1: ChlH from Chlorogloeopsis sp.



● Molecule 1: ChlH from Chlorogloeopsis sp.





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.42Å 86.99Å 198.23Å 90.00° 95.76° 90.00°	Depositor
Resolution (Å)	69.56 – 2.80 69.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	60.1 (69.56-2.80) 60.1 (69.56-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.81Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.235 , 0.255 0.232 , 0.249	Depositor DCC
R_{free} test set	2928 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16156	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.30	0/2816	0.46	0/3829
1	B	0.29	0/2805	0.47	0/3815
1	C	0.28	0/2799	0.46	0/3807
1	D	0.28	0/2744	0.46	0/3730
1	E	0.28	0/2710	0.45	0/3690
1	F	0.25	0/2628	0.43	0/3576
All	All	0.28	0/16502	0.46	0/22447

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2747	0	2754	31	0
1	B	2741	0	2741	43	0
1	C	2735	0	2737	36	0
1	D	2682	0	2696	41	0
1	E	2650	0	2680	39	0
1	F	2571	0	2603	26	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
All	All	16156	0	16211	176	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 5.

All (176) 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:504:VAL:HG23	1:B:505:PRO:HD3	1.57	0.86
1:E:473:ILE:HD13	1:F:698:HIS:CE1	2.12	0.84
1:E:474:THR:HG22	1:E:476:HIS:CE1	2.13	0.83
1:B:671:GLN:HE22	1:E:592:ARG:HH12	1.28	0.82
1:D:474:THR:HG22	1:D:476:HIS:CE1	2.14	0.81
1:A:473:ILE:HD13	1:B:698:HIS:CE1	2.19	0.77
1:A:504:VAL:HG23	1:A:505:PRO:HD3	1.65	0.76
1:C:504:VAL:HB	1:C:505:PRO:HD3	1.67	0.75
1:D:474:THR:HG23	1:D:482:LEU:HD13	1.69	0.74
1:E:474:THR:HG23	1:E:482:LEU:HD13	1.69	0.73
1:B:456:ARG:NH2	1:B:509:ARG:HH12	1.87	0.72
1:B:474:THR:HG23	1:B:482:LEU:HD13	1.73	0.71
1:B:671:GLN:HE22	1:E:592:ARG:NH1	1.91	0.69
1:C:504:VAL:HB	1:C:505:PRO:CD	2.23	0.69
1:A:579[B]:SER:OG	1:A:614:GLN:NE2	2.26	0.68
1:D:456:ARG:NH2	1:D:509:ARG:HH12	1.91	0.68
1:B:474:THR:HG22	1:B:476:HIS:NE2	2.08	0.67
1:C:473:ILE:HD13	1:D:698:HIS:CE1	2.29	0.66
1:A:698:HIS:CE1	1:B:473:ILE:HD13	2.30	0.66
1:A:456:ARG:NH2	1:A:509:ARG:HH12	1.93	0.66
1:C:456:ARG:NH2	1:C:509:ARG:HH12	1.94	0.65
1:D:566:LYS:NZ	1:D:592:ARG:HH21	1.95	0.65
1:E:438:ILE:HD13	1:E:491:GLU:HG2	1.78	0.65
1:D:566:LYS:NZ	1:D:592:ARG:NH2	2.45	0.64
1:E:698:HIS:NE2	1:F:473:ILE:HD13	2.12	0.63
1:E:474:THR:CG2	1:E:476:HIS:CE1	2.82	0.62
1:F:456:ARG:NH2	1:F:509:ARG:HH12	1.98	0.62
1:A:440:ASN:HD22	1:A:443:GLN:NE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:TRP:CD2	1:A:455:LEU:HD22	2.35	0.61
1:F:413:TRP:CD2	1:F:455:LEU:HD22	2.36	0.61
1:A:473:ILE:HD13	1:B:698:HIS:NE2	2.15	0.61
1:C:413:TRP:CD2	1:C:455:LEU:HD22	2.35	0.61
1:B:579:SER:HB2	1:B:614:GLN:NE2	2.15	0.61
1:D:413:TRP:CD2	1:D:455:LEU:HD22	2.35	0.61
1:D:627:GLU:HG2	1:D:700:THR:HG22	1.83	0.61
1:D:474:THR:CG2	1:D:476:HIS:CE1	2.84	0.61
1:B:413:TRP:CD2	1:B:455:LEU:HD22	2.37	0.60
1:D:579:SER:HB2	1:D:614:GLN:NE2	2.17	0.60
1:E:413:TRP:CD2	1:E:455:LEU:HD22	2.36	0.60
1:E:579:SER:HB2	1:E:614:GLN:NE2	2.16	0.60
1:B:590:SER:OG	1:B:593:GLN:NE2	2.34	0.60
1:F:579:SER:HB2	1:F:614:GLN:NE2	2.16	0.60
1:A:698:HIS:NE2	1:B:473:ILE:HD13	2.18	0.59
1:E:698:HIS:NE2	1:F:473:ILE:CD1	2.65	0.59
1:C:473:ILE:HD13	1:D:698:HIS:NE2	2.18	0.58
1:B:579:SER:HB2	1:B:614:GLN:HE21	1.69	0.58
1:A:456:ARG:NH2	1:A:509:ARG:NH1	2.52	0.58
1:C:579:SER:HB2	1:C:614:GLN:NE2	2.18	0.57
1:C:621:ARG:NH1	1:D:367:HIS:CD2	2.71	0.57
1:C:456:ARG:NH2	1:C:509:ARG:NH1	2.52	0.57
1:E:579:SER:HB2	1:E:614:GLN:HE21	1.68	0.57
1:F:579:SER:HB2	1:F:614:GLN:HE21	1.69	0.57
1:D:456:ARG:NH2	1:D:509:ARG:NH1	2.52	0.57
1:C:698:HIS:NE2	1:D:473:ILE:HD13	2.19	0.56
1:C:429:LEU:HD12	1:C:433:PRO:HA	1.88	0.56
1:C:579:SER:HB2	1:C:614:GLN:HE21	1.70	0.56
1:A:477:SER:HB3	1:A:483:ILE:HD11	1.87	0.56
1:B:456:ARG:NH2	1:B:509:ARG:NH1	2.52	0.55
1:C:624:PRO:O	1:C:700:THR:HG21	2.06	0.55
1:E:473:ILE:CD1	1:F:698:HIS:NE2	2.69	0.55
1:E:504:VAL:HB	1:E:505:PRO:HD3	1.88	0.55
1:F:624:PRO:O	1:F:700:THR:HG21	2.07	0.55
1:C:580:ASP:HA	1:D:362:HIS:HB2	1.89	0.55
1:D:507:ILE:HD12	1:D:537:VAL:HG11	1.89	0.55
1:F:456:ARG:NH2	1:F:509:ARG:NH1	2.55	0.55
1:D:579:SER:HB2	1:D:614:GLN:HE21	1.70	0.54
1:C:620:GLN:HE21	1:D:367:HIS:HE1	1.54	0.54
1:A:429:LEU:HD12	1:A:439:ILE:HD13	1.89	0.54
1:C:429:LEU:HD13	1:C:439:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:590:SER:OG	1:E:593:GLN:NE2	2.40	0.54
1:D:619:LEU:O	1:D:622:SER:O	2.26	0.53
1:D:566:LYS:HZ3	1:D:592:ARG:NH2	2.06	0.52
1:E:473:ILE:HD13	1:F:698:HIS:NE2	2.24	0.52
1:B:504:VAL:HB	1:B:556:ILE:HG23	1.91	0.52
1:D:478:ILE:HG12	1:D:518:PHE:HA	1.92	0.52
1:C:698:HIS:CD2	1:D:473:ILE:HD13	2.45	0.51
1:A:473:ILE:CD1	1:B:698:HIS:NE2	2.73	0.51
1:E:478:ILE:HG12	1:E:518:PHE:HA	1.91	0.51
1:C:698:HIS:CE1	1:D:473:ILE:CD1	2.94	0.51
1:E:616:LEU:HD23	1:E:649:HIS:CD2	2.45	0.51
1:D:413:TRP:CE2	1:D:455:LEU:HD22	2.46	0.51
1:F:478:ILE:HG12	1:F:518:PHE:HA	1.93	0.51
1:F:636:PRO:HG3	1:F:689:VAL:HG23	1.93	0.51
1:A:413:TRP:CE2	1:A:455:LEU:HD22	2.45	0.51
1:C:478:ILE:HG12	1:C:518:PHE:HA	1.92	0.51
1:B:478:ILE:HG12	1:B:518:PHE:HA	1.92	0.50
1:D:566:LYS:HZ3	1:D:592:ARG:HH21	1.59	0.50
1:E:474:THR:HG23	1:E:482:LEU:CD1	2.40	0.50
1:A:478:ILE:HG12	1:A:518:PHE:HA	1.92	0.50
1:B:595:SER:O	1:E:599:ASP:OD2	2.29	0.50
1:D:566:LYS:HZ2	1:D:592:ARG:NH2	2.09	0.50
1:E:413:TRP:CE2	1:E:455:LEU:HD22	2.46	0.50
1:F:413:TRP:CE2	1:F:455:LEU:HD22	2.45	0.50
1:C:413:TRP:CE2	1:C:455:LEU:HD22	2.46	0.50
1:E:507:ILE:HD12	1:E:537:VAL:HG11	1.93	0.50
1:F:616:LEU:HD23	1:F:649:HIS:CD2	2.47	0.50
1:B:413:TRP:CE2	1:B:455:LEU:HD22	2.47	0.50
1:B:671:GLN:NE2	1:E:592:ARG:NH1	2.59	0.50
1:A:579[A]:SER:HB2	1:A:614:GLN:NE2	2.28	0.49
1:B:474:THR:CG2	1:B:476:HIS:NE2	2.74	0.49
1:D:625:LEU:HD23	1:D:703:GLY:HA2	1.96	0.48
1:B:418:ARG:NH2	1:B:447:PRO:HB3	2.29	0.48
1:E:698:HIS:CD2	1:F:473:ILE:HD13	2.49	0.48
1:A:616:LEU:HD23	1:A:649:HIS:CD2	2.49	0.48
1:C:616:LEU:HD23	1:C:649:HIS:CD2	2.49	0.48
1:B:616:LEU:HD23	1:B:649:HIS:CD2	2.49	0.48
1:A:580:ASP:HA	1:B:362:HIS:HB3	1.95	0.48
1:F:428:VAL:HG22	1:F:487:ILE:HG22	1.96	0.48
1:B:633:VAL:HG22	1:B:634:PRO:HD2	1.96	0.48
1:C:598:ILE:HD11	1:C:603:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:THR:HG23	1:D:482:LEU:CD1	2.41	0.47
1:D:616:LEU:HD23	1:D:649:HIS:CD2	2.49	0.47
1:E:506:TYR:CD2	1:E:509:ARG:NH1	2.80	0.47
1:E:698:HIS:CE1	1:F:473:ILE:HD11	2.50	0.47
1:D:544:ILE:HG23	1:D:551:LEU:HD12	1.95	0.47
1:B:544:ILE:HG23	1:B:551:LEU:HD12	1.97	0.47
1:A:459:VAL:HG22	1:A:493:LEU:HD11	1.96	0.46
1:C:473:ILE:CD1	1:D:698:HIS:NE2	2.79	0.46
1:B:474:THR:HG23	1:B:482:LEU:CD1	2.43	0.46
1:C:621:ARG:HH11	1:D:367:HIS:CD2	2.32	0.46
1:B:644:PRO:HB3	1:B:697:THR:HG21	1.98	0.46
1:E:388:ILE:N	1:E:412:HIS:HE2	2.13	0.46
1:C:620:GLN:HE21	1:D:367:HIS:CE1	2.35	0.45
1:C:644:PRO:HB3	1:C:697:THR:HG21	1.98	0.45
1:F:644:PRO:HB3	1:F:697:THR:HG21	1.99	0.45
1:B:474:THR:CG2	1:B:476:HIS:CE1	2.99	0.45
1:E:545:GLU:HB2	1:E:552:LEU:HD22	1.99	0.45
1:E:698:HIS:CE1	1:F:473:ILE:CD1	2.99	0.45
1:C:473:ILE:CD1	1:D:698:HIS:CD2	2.99	0.45
1:E:647:LEU:HD11	1:E:690:ALA:HB1	1.99	0.45
1:C:475:ILE:HG12	1:D:631:PRO:HG3	1.99	0.44
1:D:504:VAL:HG13	1:D:505:PRO:HD2	2.00	0.44
1:F:612:ARG:HB2	1:F:653:VAL:HG22	1.99	0.44
1:A:698:HIS:NE2	1:B:473:ILE:CD1	2.79	0.44
1:C:545:GLU:HB2	1:C:552:LEU:HD22	1.99	0.44
1:D:644:PRO:HB3	1:D:697:THR:HG21	1.99	0.44
1:A:473:ILE:CD1	1:B:698:HIS:CD2	3.00	0.43
1:C:391:ILE:HD11	1:C:405:SER:HB3	2.00	0.43
1:A:644:PRO:HB3	1:A:697:THR:HG21	1.99	0.43
1:A:651:ILE:HG22	1:A:710:LEU:HD13	2.00	0.43
1:C:529:VAL:CG1	1:C:592:ARG:HD2	2.49	0.43
1:E:504:VAL:CB	1:E:505:PRO:HD3	2.47	0.43
1:A:440:ASN:ND2	1:A:443:GLN:NE2	2.66	0.43
1:F:545:GLU:HB2	1:F:552:LEU:HD22	1.99	0.43
1:B:474:THR:HG21	1:B:476:HIS:CE1	2.54	0.43
1:A:545:GLU:HB2	1:A:552:LEU:HD22	2.00	0.43
1:A:581:ASN:ND2	1:B:367:HIS:ND1	2.66	0.43
1:D:545:GLU:HB2	1:D:552:LEU:HD22	2.00	0.43
1:F:505:PRO:O	1:F:507:ILE:HG13	2.19	0.43
1:E:393:ILE:HD11	1:E:705:GLU:HB3	2.01	0.42
1:B:477:SER:HB3	1:B:483:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:LEU:HD22	1:E:497:LEU:HD21	2.00	0.42
1:E:473:ILE:CD1	1:F:698:HIS:CE1	2.94	0.42
1:B:651:ILE:HG22	1:B:710:LEU:HD13	2.02	0.42
1:C:362:HIS:HB2	1:D:580:ASP:HA	2.01	0.42
1:B:431:LYS:HE3	1:B:487:ILE:HD11	2.00	0.42
1:E:446:PRO:HD2	1:E:449:ILE:HD12	2.02	0.42
1:B:545:GLU:HB2	1:B:552:LEU:HD22	2.00	0.41
1:D:651:ILE:HG22	1:D:710:LEU:HD13	2.02	0.41
1:D:446:PRO:HA	1:D:447:PRO:HD3	1.98	0.41
1:A:446:PRO:HA	1:A:447:PRO:HD3	1.98	0.41
1:C:633:VAL:HG22	1:C:634:PRO:HD2	2.01	0.41
1:E:406:ILE:HD13	1:E:558:ILE:HD11	2.03	0.41
1:A:531:ASN:ND2	1:C:539:GLU:OE2	2.54	0.41
1:E:561:GLU:HB2	1:E:586:ALA:HA	2.02	0.41
1:A:475:ILE:HG12	1:B:631:PRO:HG3	2.01	0.41
1:C:642:ARG:HD2	1:C:642:ARG:HA	1.96	0.41
1:B:599:ASP:OD2	1:E:595:SER:O	2.39	0.41
1:C:529:VAL:HG12	1:C:591:ILE:HD11	2.03	0.41
1:F:647:LEU:HD23	1:F:694:LEU:HB2	2.02	0.41
1:B:439:ILE:O	1:B:443:GLN:HG3	2.21	0.41
1:A:446:PRO:HD2	1:A:449:ILE:HD12	2.02	0.40
1:A:631:PRO:HG3	1:B:475:ILE:HG12	2.02	0.40
1:B:456:ARG:HH21	1:B:509:ARG:HH12	1.61	0.40
1:F:609:HIS:CD2	1:F:610:GLU:OE2	2.75	0.40
1:E:612:ARG:HB2	1:E:653:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	341/368 (93%)	326 (96%)	15 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	339/368 (92%)	321 (95%)	18 (5%)	0	100	100
1	C	338/368 (92%)	320 (95%)	17 (5%)	1 (0%)	37	67
1	D	327/368 (89%)	308 (94%)	16 (5%)	3 (1%)	14	42
1	E	329/368 (89%)	320 (97%)	8 (2%)	1 (0%)	37	67
1	F	316/368 (86%)	308 (98%)	7 (2%)	1 (0%)	37	67
All	All	1990/2208 (90%)	1903 (96%)	81 (4%)	6 (0%)	37	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	504	VAL
1	E	504	VAL
1	F	506	TYR
1	D	505	PRO
1	D	504	VAL
1	D	623	ILE

5.3.2 Protein sidechains [i](#)

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	307/328 (94%)	297 (97%)	10 (3%)	33	67
1	B	306/328 (93%)	292 (95%)	14 (5%)	23	55
1	C	305/328 (93%)	296 (97%)	9 (3%)	36	70
1	D	300/328 (92%)	289 (96%)	11 (4%)	29	63
1	E	295/328 (90%)	287 (97%)	8 (3%)	40	74
1	F	287/328 (88%)	278 (97%)	9 (3%)	35	69
All	All	1800/1968 (92%)	1739 (97%)	61 (3%)	32	66

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	A	429	LEU
1	A	437	ASP
1	A	504	VAL
1	A	583	VAL
1	A	592	ARG
1	A	593	GLN
1	A	656	HIS
1	A	667	GLU
1	A	697	THR
1	B	364	HIS
1	B	390	PHE
1	B	391	ILE
1	B	429	LEU
1	B	504	VAL
1	B	583	VAL
1	B	593	GLN
1	B	621	ARG
1	B	633	VAL
1	B	640	ASP
1	B	641	LEU
1	B	656	HIS
1	B	697	THR
1	B	717	MET
1	C	361	SER
1	C	362	HIS
1	C	364	HIS
1	C	429	LEU
1	C	583	VAL
1	C	600	GLN
1	C	633	VAL
1	C	656	HIS
1	C	697	THR
1	D	362	HIS
1	D	364	HIS
1	D	365	HIS
1	D	429	LEU
1	D	440	ASN
1	D	583	VAL
1	D	593	GLN
1	D	600	GLN
1	D	622	SER
1	D	656	HIS

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Mol	Chain	Res	Type
1	D	697	THR
1	E	393	ILE
1	E	418	ARG
1	E	504	VAL
1	E	583	VAL
1	E	656	HIS
1	E	669	GLN
1	E	670	ASP
1	E	671	GLN
1	F	437	ASP
1	F	583	VAL
1	F	600	GLN
1	F	605	ASP
1	F	633	VAL
1	F	656	HIS
1	F	671	GLN
1	F	697	THR
1	F	717	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	GLN
1	A	581	ASN
1	A	609	HIS
1	B	581	ASN
1	B	593	GLN
1	B	609	HIS
1	B	671	GLN
1	C	571	HIS
1	C	581	ASN
1	C	620	GLN
1	D	571	HIS
1	D	581	ASN
1	D	609	HIS
1	D	620	GLN
1	E	440	ASN
1	E	476	HIS
1	F	593	GLN
1	F	609	HIS
1	F	671	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	B	801	-	4,4,4	0.17	0	6,6,6	0.34	0
2	PO4	A	801	-	4,4,4	0.24	0	6,6,6	0.29	0
2	PO4	C	801	-	4,4,4	0.21	0	6,6,6	0.29	0
2	PO4	F	801	-	4,4,4	0.12	0	6,6,6	0.30	0
2	PO4	D	801	-	4,4,4	0.21	0	6,6,6	0.28	0
2	PO4	E	801	-	4,4,4	0.17	0	6,6,6	0.29	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	342/368 (92%)	0.47	25 (7%) 22 17	23, 57, 83, 98	8 (2%)
1	B	342/368 (92%)	0.68	28 (8%) 19 14	39, 63, 93, 100	5 (1%)
1	C	342/368 (92%)	0.78	39 (11%) 11 9	49, 71, 105, 116	3 (0%)
1	D	335/368 (91%)	1.55	81 (24%) 2 2	66, 86, 116, 131	3 (0%)
1	E	331/368 (89%)	1.08	43 (12%) 9 7	50, 73, 118, 125	0
1	F	320/368 (86%)	1.50	77 (24%) 2 2	73, 96, 134, 144	0
All	All	2012/2208 (91%)	1.00	293 (14%) 7 6	23, 74, 116, 144	19 (0%)

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	391	ILE	8.3
1	D	500	PRO	7.3
1	F	394	ALA	6.7
1	D	361	SER	6.3
1	A	361	SER	6.1
1	F	487	ILE	6.1
1	A	370	GLY	5.9
1	F	400	LEU	5.7
1	B	361	SER	5.4
1	C	361	SER	5.2
1	C	370	GLY	5.1
1	D	370	GLY	5.1
1	B	390	PHE	5.1
1	A	359	GLY	5.0
1	D	494	ALA	5.0
1	F	663	TYR	4.9
1	C	365	HIS	4.7
1	D	394	ALA	4.7
1	D	393	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	362	HIS	4.6
1	E	504	VAL	4.5
1	D	497	LEU	4.5
1	E	472	GLY	4.4
1	A	362	HIS	4.4
1	E	501	ASN	4.4
1	C	368	SER	4.4
1	C	358	MET	4.3
1	D	674	VAL	4.3
1	F	505	PRO	4.1
1	D	400	LEU	4.1
1	A	367	HIS	4.0
1	D	365	HIS	3.9
1	B	718	GLY	3.9
1	D	359	GLY	3.9
1	A	504	VAL	3.9
1	C	367	HIS	3.8
1	D	504	VAL	3.8
1	D	362	HIS	3.8
1	B	367	HIS	3.8
1	B	497	LEU	3.8
1	A	500	PRO	3.7
1	F	478	ILE	3.7
1	C	504	VAL	3.7
1	D	506	TYR	3.6
1	D	358	MET	3.6
1	C	640	ASP	3.6
1	A	360	SER	3.6
1	F	401	THR	3.6
1	C	390	PHE	3.6
1	F	504	VAL	3.5
1	D	426	MET	3.5
1	D	718	GLY	3.5
1	F	426	MET	3.5
1	D	367	HIS	3.5
1	F	717	MET	3.5
1	F	666	ARG	3.4
1	D	672	ILE	3.4
1	E	393	ILE	3.4
1	D	667	GLU	3.4
1	B	504	VAL	3.4
1	A	365	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	438	ILE	3.3
1	D	392	ASP	3.3
1	E	593	GLN	3.3
1	E	444	THR	3.3
1	A	639	GLU	3.3
1	E	578	PHE	3.3
1	C	500	PRO	3.3
1	F	667	GLU	3.2
1	D	521	ARG	3.2
1	D	429	LEU	3.2
1	E	505	PRO	3.2
1	F	439	ILE	3.2
1	D	707	VAL	3.2
1	C	359	GLY	3.2
1	B	358	MET	3.2
1	F	497	LEU	3.2
1	F	431	LYS	3.1
1	F	536	ILE	3.1
1	A	495	GLU	3.1
1	D	444	THR	3.1
1	E	487	ILE	3.1
1	F	418	ARG	3.1
1	F	494	ALA	3.1
1	A	718	GLY	3.1
1	B	359	GLY	3.1
1	C	433	PRO	3.1
1	C	366	HIS	3.0
1	B	521	ARG	3.0
1	C	369	SER	3.0
1	B	500	PRO	3.0
1	D	663	TYR	3.0
1	B	501	ASN	3.0
1	C	435	LYS	3.0
1	A	390	PHE	3.0
1	B	370	GLY	3.0
1	E	640	ASP	2.9
1	F	454	VAL	2.9
1	C	443	GLN	2.9
1	F	533	GLY	2.9
1	E	500	PRO	2.9
1	E	681	GLU	2.8
1	C	470	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	670	ASP	2.8
1	F	718	GLY	2.8
1	B	672	ILE	2.8
1	F	496	SER	2.8
1	D	575	VAL	2.8
1	F	715	THR	2.8
1	E	506	TYR	2.8
1	C	434	GLY	2.8
1	D	523	LEU	2.8
1	F	674	VAL	2.8
1	D	593	GLN	2.8
1	E	447	PRO	2.8
1	F	506	TYR	2.8
1	D	360	SER	2.7
1	E	448	GLU	2.7
1	A	358	MET	2.7
1	D	673	LYS	2.7
1	B	578	PHE	2.7
1	F	442	PHE	2.7
1	C	498	LYS	2.7
1	D	431	LYS	2.7
1	E	431	LYS	2.7
1	F	547	TRP	2.7
1	A	573	ASP	2.6
1	F	595	SER	2.6
1	D	623	ILE	2.6
1	F	452	LYS	2.6
1	C	718	GLY	2.6
1	B	712	GLU	2.6
1	D	621	ARG	2.6
1	B	412	HIS	2.6
1	F	412	HIS	2.6
1	E	585	GLY	2.6
1	F	449	ILE	2.6
1	C	360	SER	2.6
1	F	422	GLU	2.6
1	B	506	TYR	2.6
1	D	600	GLN	2.6
1	A	578	PHE	2.6
1	D	415	ALA	2.6
1	D	613	HIS	2.6
1	C	444	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	360	SER	2.5
1	F	661	TRP	2.5
1	D	641	LEU	2.5
1	D	505	PRO	2.5
1	E	581	ASN	2.5
1	F	433	PRO	2.5
1	C	684	ARG	2.5
1	F	593	GLN	2.5
1	D	550	ALA	2.5
1	F	518	PHE	2.5
1	F	438	ILE	2.5
1	D	499	SER	2.5
1	E	450	LEU	2.5
1	F	421	PHE	2.5
1	E	449	ILE	2.5
1	E	553	SER	2.5
1	E	595	SER	2.5
1	F	429	LEU	2.5
1	C	362	HIS	2.5
1	F	677	LYS	2.5
1	C	503	GLY	2.5
1	C	700	THR	2.5
1	D	680	VAL	2.4
1	C	412	HIS	2.4
1	D	569	THR	2.4
1	B	675	ARG	2.4
1	A	499	SER	2.4
1	B	593	GLN	2.4
1	E	489	TYR	2.4
1	F	448	GLU	2.4
1	B	505	PRO	2.4
1	E	435	LYS	2.4
1	C	364	HIS	2.4
1	E	600	GLN	2.4
1	D	522	ILE	2.4
1	B	701	THR	2.3
1	E	684	ARG	2.3
1	B	364	HIS	2.3
1	D	653	VAL	2.3
1	B	369[A]	SER	2.3
1	D	597	TYR	2.3
1	A	670	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	437	ASP	2.3
1	D	552	LEU	2.3
1	D	433	PRO	2.3
1	D	439	ILE	2.3
1	F	703	GLY	2.3
1	A	431	LYS	2.3
1	A	714	THR	2.3
1	F	474	THR	2.3
1	D	675	ARG	2.3
1	F	627	GLU	2.3
1	D	443	GLN	2.3
1	F	576	VAL	2.3
1	F	707	VAL	2.3
1	D	449	ILE	2.3
1	D	478	ILE	2.3
1	E	507	ILE	2.3
1	F	591	ILE	2.3
1	F	489	TYR	2.3
1	D	536	ILE	2.3
1	D	513	TRP	2.3
1	A	717	MET	2.2
1	C	502	GLU	2.2
1	C	601	TYR	2.2
1	D	626	ILE	2.2
1	D	694	LEU	2.2
1	F	493	LEU	2.2
1	E	499	SER	2.2
1	F	403	SER	2.2
1	F	684	ARG	2.2
1	E	671	GLN	2.2
1	C	630	ALA	2.2
1	F	664	LEU	2.2
1	F	592	ARG	2.2
1	D	403	SER	2.2
1	E	495	GLU	2.2
1	C	501	ASN	2.2
1	F	563	GLN	2.2
1	D	566	LYS	2.2
1	F	695	LYS	2.2
1	A	472	GLY	2.2
1	F	447	PRO	2.2
1	F	416	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	620	GLN	2.2
1	F	654	PHE	2.2
1	F	498	LYS	2.2
1	D	688	LEU	2.2
1	D	503	GLY	2.2
1	F	668	GLY	2.2
1	D	622	SER	2.1
1	D	665	SER	2.1
1	A	412	HIS	2.1
1	D	640	ASP	2.1
1	D	498	LYS	2.1
1	F	671	GLN	2.1
1	D	648	LEU	2.1
1	E	429	LEU	2.1
1	E	718	GLY	2.1
1	E	446	PRO	2.1
1	D	562	ILE	2.1
1	E	396	PHE	2.1
1	E	617	TYR	2.1
1	F	600	GLN	2.1
1	F	709	GLN	2.1
1	F	530	GLY	2.1
1	B	363	HIS	2.1
1	F	682	THR	2.1
1	B	529	VAL	2.1
1	C	478	ILE	2.1
1	D	556	ILE	2.1
1	D	716	ASN	2.1
1	E	674	VAL	2.1
1	F	529	VAL	2.1
1	F	623	ILE	2.1
1	C	490	LEU	2.1
1	E	467	LEU	2.1
1	E	418	ARG	2.1
1	F	417	ALA	2.1
1	F	696	ARG	2.1
1	D	485	PRO	2.1
1	C	431	LYS	2.1
1	D	435	LYS	2.1
1	F	435	LYS	2.1
1	D	438	ILE	2.1
1	F	598	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	468	GLN	2.1
1	C	506	TYR	2.1
1	D	601	TYR	2.1
1	D	662	ALA	2.1
1	F	561	GLU	2.0
1	C	697	THR	2.0
1	C	391	ILE	2.0
1	C	487	ILE	2.0
1	F	532	ILE	2.0
1	A	369	SER	2.0
1	D	660	PHE	2.0
1	D	453	LEU	2.0
1	D	596	ARG	2.0
1	F	601	TYR	2.0
1	D	484	ALA	2.0
1	F	434	GLY	2.0
1	E	475	ILE	2.0
1	E	454	VAL	2.0
1	F	587	LEU	2.0
1	F	658	LEU	2.0
1	A	436	ARG	2.0
1	B	403	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	F	801	5/5	0.70	0.11	128,128,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	E	801	5/5	0.82	0.12	109,109,109,109	0
2	PO4	D	801	5/5	0.82	0.15	110,110,110,110	0
2	PO4	B	801	5/5	0.85	0.10	78,78,78,78	0
2	PO4	C	801	5/5	0.86	0.10	84,84,84,84	0
2	PO4	A	801	5/5	0.92	0.07	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.