



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:36 PM UTC

PDB ID : 5FLF / pdb_00005ff
Title : DISEASE LINKED MUTATION IN FGFR
Authors : Thiyagarajan, N.; Bunney, T.D.; Katan, M.
Deposited on : 2015-10-26
Resolution : 2.58 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

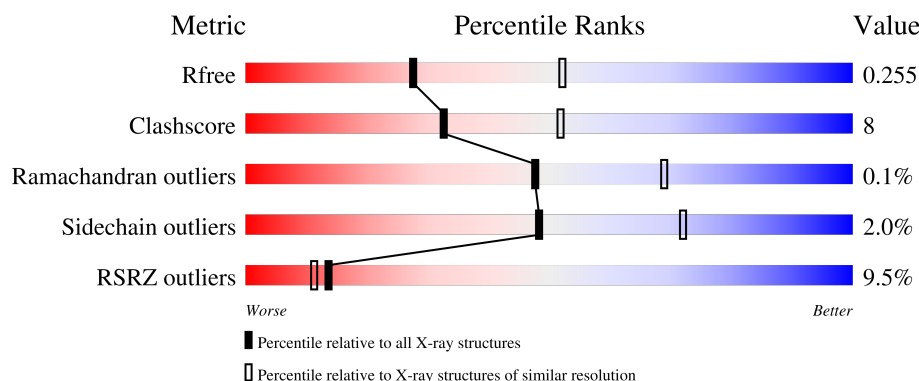
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	310	7% 81% 14% • 5%
1	B	310	5% 78% 15% • 6%
1	C	310	5% 74% 17% • 9%
1	D	310	6% 77% 16% 6%
1	E	310	21% 67% 14% • 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	D	1773	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11786 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 FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2358	1501	402	438	17			
1	B	292	Total	C	N	O	S	0	4	0
			2350	1496	404	432	18			
1	C	283	Total	C	N	O	S	0	2	0
			2263	1440	391	414	18			
1	D	290	Total	C	N	O	S	0	1	0
			2312	1470	398	427	17			
1	E	258	Total	C	N	O	S	0	0	0
			2045	1304	353	371	17			

There are 25 discrepancies between the modelled and reference sequences:

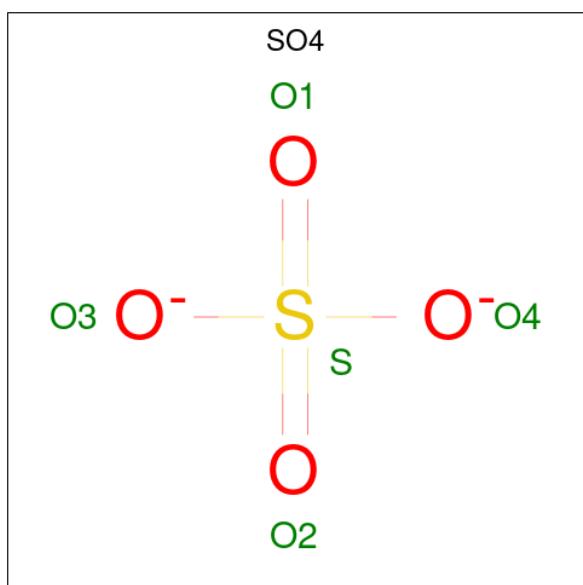
Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	-	expression tag	UNP P11362
A	457	VAL	-	expression tag	UNP P11362
A	488	ALA	CYS	conflict	UNP P11362
A	584	SER	CYS	conflict	UNP P11362
A	675	GLY	ARG	engineered mutation	UNP P11362
B	456	MET	-	expression tag	UNP P11362
B	457	VAL	-	expression tag	UNP P11362
B	488	ALA	CYS	conflict	UNP P11362
B	584	SER	CYS	conflict	UNP P11362
B	675	GLY	ARG	engineered mutation	UNP P11362
C	456	MET	-	expression tag	UNP P11362
C	457	VAL	-	expression tag	UNP P11362
C	488	ALA	CYS	conflict	UNP P11362
C	584	SER	CYS	conflict	UNP P11362
C	675	GLY	ARG	engineered mutation	UNP P11362
D	456	MET	-	expression tag	UNP P11362
D	457	VAL	-	expression tag	UNP P11362
D	488	ALA	CYS	conflict	UNP P11362
D	584	SER	CYS	conflict	UNP P11362

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Chain	Residue	Modelled	Actual	Comment	Reference
D	675	GLY	ARG	engineered mutation	UNP P11362
E	456	MET	-	expression tag	UNP P11362
E	457	VAL	-	expression tag	UNP P11362
E	488	ALA	CYS	conflict	UNP P11362
E	584	SER	CYS	conflict	UNP P11362
E	675	GLY	ARG	engineered mutation	UNP P11362

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

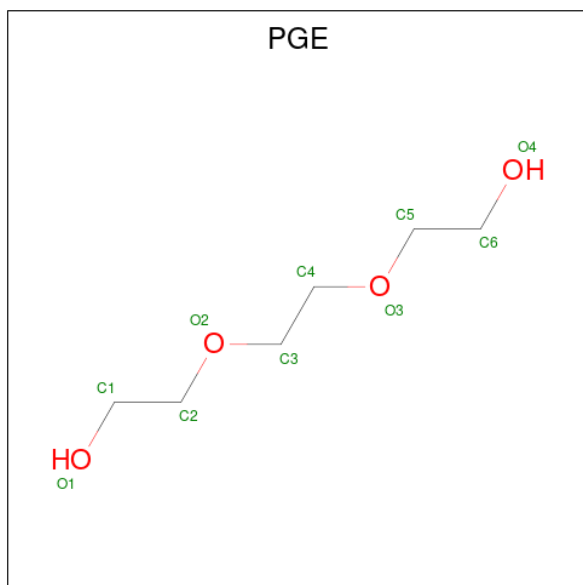


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	3	Total	Cl	0	0
			3	3		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

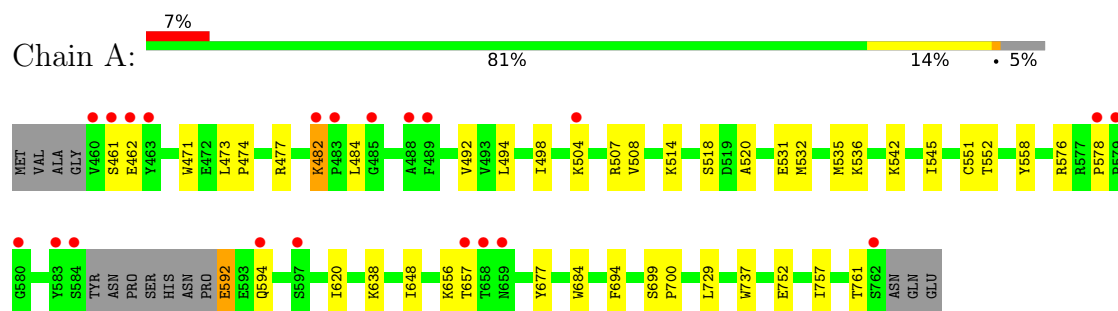
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	101	Total	O	0	0
			101	101		
6	C	70	Total	O	0	0
			70	70		
6	D	94	Total	O	0	0
			94	94		
6	E	28	Total	O	0	0
			28	28		

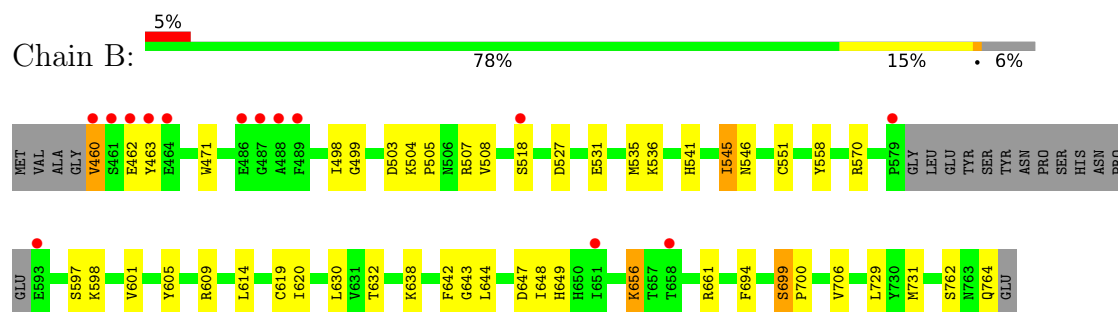
3 Residue-property plots [i](#)

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.

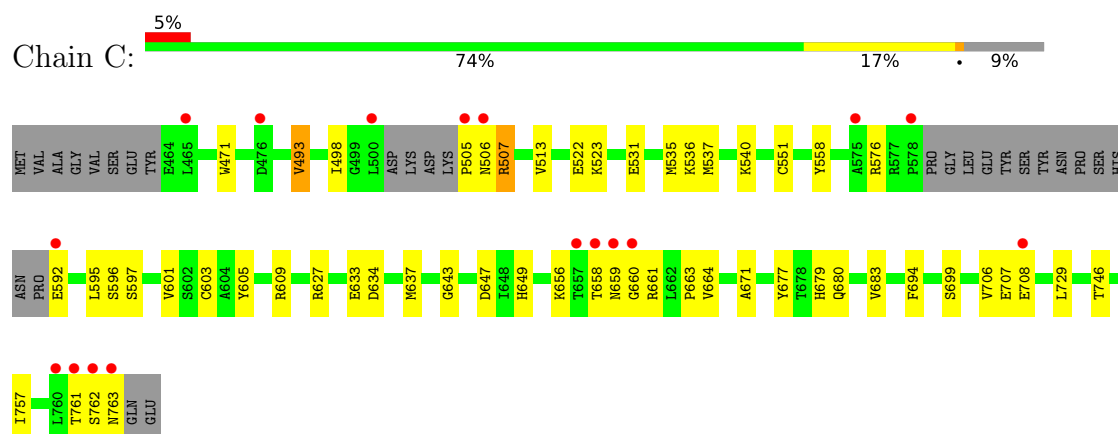
• Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1



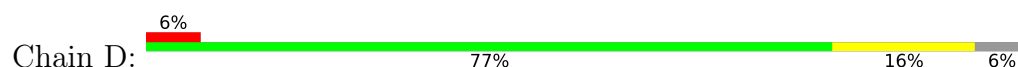
• Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1

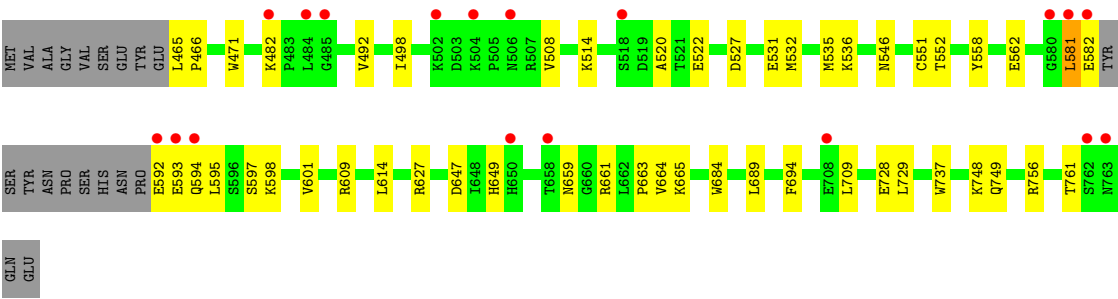


• Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1

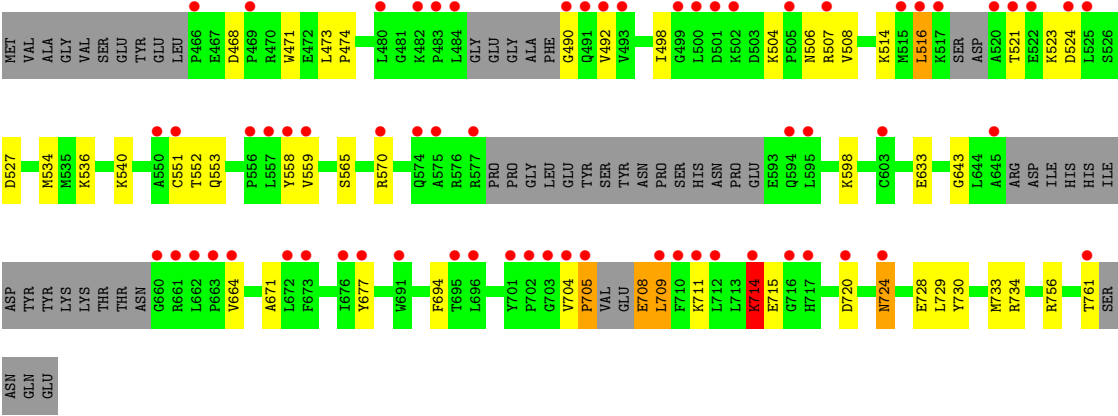


• Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1





● Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.26Å 152.28Å 195.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.06 – 2.58 71.06 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.5 (71.06-2.58) 97.5 (71.06-2.58)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.194 , 0.255 0.202 , 0.255	Depositor DCC
R_{free} test set	3482 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11786	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PGE, ACT, CL

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	0.29	0/2408	0.73	0/3254
1	B	0.32	0/2409	0.79	6/3256 (0.2%)
1	C	0.29	0/2315	0.74	2/3125 (0.1%)
1	D	0.30	0/2360	0.75	1/3189 (0.0%)
1	E	0.31	0/2083	0.83	3/2808 (0.1%)
All	All	0.30	0/11575	0.77	12/15632 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	708	GLU	N-CA-C	-7.16	104.53	113.20
1	B	642	PHE	N-CA-C	7.01	120.78	112.93
1	B	643	GLY	N-CA-C	6.69	122.25	114.16
1	B	699	SER	CA-C-N	6.37	126.40	119.90
1	B	699	SER	C-N-CA	6.37	126.40	119.90
1	E	709	LEU	N-CA-C	6.03	117.52	111.07
1	B	462	GLU	N-CA-C	-5.88	106.73	114.31
1	D	581	LEU	N-CA-C	5.72	117.97	108.13
1	B	644	LEU	N-CA-C	-5.32	106.81	113.72
1	E	714	LYS	N-CA-C	-5.17	105.82	111.82
1	C	699	SER	CA-C-N	5.11	125.11	119.89
1	C	699	SER	C-N-CA	5.11	125.11	119.89

There are no chirality outliers.

There are no planarity outliers.

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	2358	0	2365	32	0
1	B	2350	0	2369	27	0
1	C	2263	0	2287	52	0
1	D	2312	0	2330	40	0
1	E	2045	0	2077	45	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	25	0	0	0	0
2	E	5	0	0	0	0
3	A	4	0	3	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
5	C	10	0	14	5	0
5	D	30	0	42	2	0
6	A	71	0	0	4	0
6	B	101	0	0	3	0
6	C	70	0	0	2	0
6	D	94	0	0	2	0
6	E	28	0	0	1	0
All	All	11786	0	11487	181	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 8.

All (181) 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:E:504:LYS:CD	1:E:507:ARG:NH1	1.76	1.48
1:E:504:LYS:HD3	1:E:507:ARG:NH1	1.05	1.36
1:E:504:LYS:HD3	1:E:507:ARG:CZ	1.60	1.30
1:C:659:ASN:ND2	1:D:522:GLU:OE1	1.65	1.29
1:E:504:LYS:NZ	1:E:507:ARG:HH12	1.31	1.28
1:C:659:ASN:OD1	1:D:522:GLU:HB2	1.31	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:LYS:CE	1:E:507:ARG:HH12	1.61	1.11
1:A:504:LYS:HD3	1:A:507:ARG:HD3	1.20	1.11
1:A:504:LYS:NZ	1:A:507:ARG:HH11	1.50	1.09
1:A:504:LYS:NZ	1:A:507:ARG:NH1	2.03	1.04
1:E:504:LYS:CE	1:E:507:ARG:NH1	2.19	0.98
1:E:504:LYS:HD3	1:E:507:ARG:HH11	1.25	0.95
1:A:504:LYS:HZ3	1:A:507:ARG:NH1	1.62	0.94
1:C:592:GLU:N	6:C:2031:HOH:O	1.99	0.93
1:E:504:LYS:NZ	1:E:507:ARG:NH1	2.17	0.93
1:A:504:LYS:HZ2	1:A:507:ARG:HH11	0.97	0.91
1:E:504:LYS:HZ3	1:E:507:ARG:HH12	1.15	0.89
1:C:659:ASN:OD1	1:D:522:GLU:CB	2.21	0.88
1:C:596:SER:HB2	1:C:763:ASN:HB3	1.54	0.88
1:A:504:LYS:CD	1:A:507:ARG:HD3	2.06	0.85
1:A:504:LYS:HD3	1:A:507:ARG:CD	2.05	0.84
1:C:596:SER:HB2	1:C:763:ASN:CB	2.12	0.80
1:C:659:ASN:CG	1:D:522:GLU:HB2	2.11	0.75
1:E:730:TYR:HA	1:E:733:MET:HE3	1.70	0.73
1:C:596:SER:CB	1:C:763:ASN:HB3	2.19	0.72
1:E:504:LYS:CD	1:E:507:ARG:CZ	2.41	0.72
1:E:534:MET:HG2	1:E:643:GLY:HA2	1.73	0.70
1:C:659:ASN:HD21	1:D:522:GLU:HB3	1.58	0.68
1:D:728:GLU:OE2	1:D:756:ARG:NH2	2.27	0.67
1:C:659:ASN:CG	1:C:660:GLY:H	2.02	0.67
1:D:627:ARG:HH21	1:D:663:PRO:HG2	1.59	0.66
1:A:518:SER:O	6:A:2012:HOH:O	2.14	0.65
1:C:523:LYS:NZ	1:D:659:ASN:O	2.30	0.65
1:E:514:LYS:HB2	1:E:559:VAL:HB	1.79	0.64
1:E:728:GLU:OE2	1:E:756:ARG:NH2	2.31	0.64
1:C:659:ASN:CG	1:C:660:GLY:N	2.56	0.64
1:A:492:VAL:HG22	1:A:514:LYS:HG2	1.80	0.63
1:D:664:VAL:HG12	1:D:709:LEU:HD23	1.81	0.63
1:D:647:ASP:OD1	1:D:649:HIS:ND1	2.27	0.62
1:C:659:ASN:HD21	1:D:522:GLU:CB	2.13	0.61
1:B:731:MET:SD	6:B:2083:HOH:O	2.56	0.61
1:D:748:LYS:HD3	5:D:1770:PGE:H32	1.81	0.61
1:A:520:ALA:HB3	1:B:706:VAL:HG21	1.83	0.60
1:A:551:CYS:HB2	1:A:558:TYR:HB2	1.84	0.59
1:B:647:ASP:OD1	1:B:649[B]:HIS:ND1	2.31	0.59
1:E:704:VAL:O	1:E:708:GLU:N	2.35	0.59
1:C:664:VAL:HG21	1:C:706:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:ASP:OD2	1:D:661:ARG:NH2	2.37	0.58
1:E:473:LEU:HD12	1:E:474:PRO:HD2	1.86	0.58
1:A:531:GLU:HG2	1:A:535:MET:HE2	1.85	0.58
1:C:656:LYS:HB3	1:C:677:TYR:HE2	1.69	0.58
1:C:683:VAL:HG21	5:C:1765:PGE:H5	1.86	0.57
1:B:531:GLU:HG2	1:B:535:MET:HE2	1.87	0.57
1:E:504:LYS:HZ3	1:E:507:ARG:NH1	1.89	0.56
1:E:724:ASN:OD1	1:E:724:ASN:N	2.37	0.56
1:D:492:VAL:HG22	1:D:514:LYS:HG2	1.86	0.56
1:E:504:LYS:CE	1:E:507:ARG:CZ	2.82	0.56
1:C:523:LYS:HE2	1:C:661:ARG:HD3	1.87	0.56
1:D:531:GLU:HG2	1:D:535:MET:HE2	1.87	0.55
1:E:521:THR:HG22	1:E:523:LYS:H	1.71	0.55
1:A:542:LYS:NZ	6:A:2020:HOH:O	2.39	0.55
1:E:711:LYS:O	1:E:715:GLU:HB2	2.06	0.55
1:B:460:VAL:N	6:B:2001:HOH:O	2.40	0.55
1:A:545:ILE:HG12	1:A:638:LYS:HB3	1.88	0.54
1:A:620:ILE:HD11	1:A:648:ILE:HD13	1.89	0.54
1:C:659:ASN:ND2	1:D:522:GLU:CB	2.71	0.54
1:C:658:THR:HG22	1:C:659:ASN:N	2.23	0.54
1:D:609:ARG:NH2	6:D:2044:HOH:O	2.40	0.54
1:E:504:LYS:HE2	1:E:507:ARG:HH22	1.72	0.53
1:B:527:ASP:OD2	1:B:661:ARG:NH2	2.29	0.53
1:E:711:LYS:HA	1:E:714:LYS:HB2	1.89	0.53
1:C:634:ASP:OD1	1:C:634:ASP:N	2.42	0.53
1:C:576:ARG:HD3	1:C:595:LEU:HD21	1.90	0.53
1:C:659:ASN:ND2	1:D:522:GLU:HB3	2.23	0.53
1:C:659:ASN:CG	1:D:522:GLU:CB	2.79	0.53
1:B:598:LYS:HD3	1:B:764:GLN:HA	1.92	0.52
1:A:752:GLU:OE2	1:C:609:ARG:NH1	2.42	0.52
1:C:627[A]:ARG:HH21	1:C:663:PRO:HG2	1.74	0.52
1:B:620[A]:ILE:HD11	1:B:648:ILE:HD13	1.92	0.52
1:E:504:LYS:HE2	1:E:507:ARG:NH2	2.25	0.52
1:A:473:LEU:HD12	1:A:474:PRO:HD2	1.92	0.51
6:A:2013:HOH:O	1:B:570:ARG:NH1	2.43	0.51
1:D:546:ASN:HB3	1:D:562:GLU:HG3	1.92	0.51
1:E:551:CYS:HB2	1:E:558:TYR:HB2	1.91	0.51
1:B:498:ILE:HG12	1:B:508:VAL:HG12	1.92	0.51
1:C:707:GLU:OE1	1:C:707:GLU:N	2.32	0.51
1:C:551:CYS:HB2	1:C:558:TYR:HB2	1.93	0.51
1:A:656:LYS:HG3	1:A:657:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ILE:O	1:A:761:THR:OG1	2.24	0.51
1:C:659:ASN:CG	1:D:522:GLU:OE1	2.47	0.50
1:E:468:ASP:OD1	1:E:468:ASP:N	2.44	0.50
1:C:531:GLU:HG2	1:C:535:MET:HE2	1.94	0.49
1:A:594:GLN:H	1:A:594:GLN:CD	2.19	0.49
1:E:490:GLY:HA2	1:E:516:LEU:HA	1.94	0.49
1:C:493:VAL:HG13	1:C:513:VAL:HB	1.95	0.49
1:D:749:GLN:HE21	5:D:1770:PGE:H52	1.78	0.49
1:B:541:HIS:H	1:B:546[B]:ASN:HD21	1.59	0.49
1:C:656:LYS:HB3	1:C:677:TYR:CE2	2.48	0.48
1:E:504:LYS:HZ2	1:E:507:ARG:HH12	1.49	0.48
1:E:705:PRO:C	1:E:709:LEU:H	2.21	0.48
1:A:656:LYS:HB3	1:A:677:TYR:HE2	1.79	0.48
1:D:598:LYS:HG3	1:D:761[B]:THR:HG23	1.96	0.48
1:D:609:ARG:NH1	6:D:2026:HOH:O	2.46	0.48
1:D:532:MET:HE1	1:D:552:THR:HG21	1.96	0.47
1:E:730:TYR:CZ	1:E:734:ARG:HD3	2.49	0.47
1:B:503:ASP:OD1	1:B:503:ASP:N	2.47	0.47
1:E:504:LYS:CD	1:E:507:ARG:HH11	1.97	0.47
1:E:714:LYS:HD3	1:E:714:LYS:HA	1.49	0.47
1:D:498:ILE:HG12	1:D:508:VAL:HG12	1.97	0.47
1:D:465:LEU:HD12	1:D:466:PRO:HD2	1.97	0.47
1:D:551:CYS:HB2	1:D:558:TYR:HB2	1.95	0.47
1:E:498:ILE:O	1:E:507:ARG:O	2.33	0.47
1:C:706:VAL:HG21	1:D:520:ALA:HB3	1.97	0.47
1:C:746:THR:HA	5:C:1765:PGE:H52	1.97	0.47
1:A:578:PRO:HG3	1:A:594:GLN:HG2	1.96	0.46
1:A:477:ARG:HA	1:A:477:ARG:HD3	1.69	0.46
1:C:531:GLU:HB2	1:C:643:GLY:HA2	1.97	0.46
1:C:679:HIS:HB3	5:C:1765:PGE:H32	1.96	0.46
1:E:552:THR:OG1	1:E:553:GLN:OE1	2.22	0.46
1:A:484:LEU:HD21	1:A:494:LEU:HB2	1.98	0.45
1:C:540:LYS:HE3	1:C:540:LYS:HB2	1.69	0.45
1:A:482:LYS:HE3	1:A:494:LEU:HD23	1.98	0.45
1:B:471:TRP:CD1	1:B:536:LYS:HE2	2.51	0.45
1:B:460:VAL:HG13	1:B:463:TYR:CD2	2.51	0.45
1:D:694:PHE:CZ	1:D:729:LEU:HD13	2.52	0.45
1:A:699:SER:HA	1:A:700:PRO:HD3	1.85	0.45
1:B:499:GLY:HA2	1:B:505:PRO:HA	1.99	0.45
1:B:694:PHE:CZ	1:B:729:LEU:HD13	2.52	0.45
1:B:504:LYS:HD3	1:B:507:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:LYS:NZ	1:C:671:ALA:O	2.42	0.45
1:B:551:CYS:HB2	1:B:558:TYR:HB2	1.99	0.45
1:B:605:TYR:CZ	1:B:609:ARG:HD2	2.51	0.45
1:C:757:ILE:O	1:C:761:THR:OG1	2.29	0.45
1:C:746:THR:HG22	5:C:1765:PGE:H42	1.99	0.44
1:E:671:ALA:HB1	1:E:677:TYR:CE2	2.51	0.44
1:C:505:PRO:HB2	1:C:506:ASN:H	1.56	0.44
1:C:762:SER:O	1:C:762:SER:OG	2.32	0.44
1:E:524:ASP:HA	1:E:527:ASP:HB2	1.99	0.44
6:A:2065:HOH:O	1:C:605:TYR:OH	2.21	0.44
1:B:545:ILE:HD11	1:B:630:LEU:HD12	1.98	0.44
1:C:603[B]:CYS:SG	1:C:637:MET:HE3	2.57	0.44
1:C:694:PHE:CZ	1:C:729:LEU:HD13	2.53	0.44
1:A:471:TRP:CD1	1:A:536:LYS:HE2	2.53	0.43
1:B:656:LYS:HA	1:B:656:LYS:HD2	1.67	0.43
1:C:680:GLN:HA	5:C:1765:PGE:H6	1.99	0.43
1:E:720:ASP:OD1	1:E:720:ASP:N	2.47	0.43
1:D:597:SER:O	1:D:601:VAL:HG23	2.18	0.43
1:D:665:LYS:HG2	1:D:709:LEU:HD22	2.01	0.43
1:E:523:LYS:O	1:E:523:LYS:HD2	2.18	0.43
1:A:498:ILE:HA	1:A:508:VAL:HG12	2.01	0.43
1:A:532:MET:HE1	1:A:552:THR:HG21	1.99	0.43
1:D:482:LYS:H	1:D:482:LYS:HG2	1.51	0.43
1:C:597:SER:O	1:C:601:VAL:HG23	2.19	0.43
1:C:507:ARG:CZ	1:C:507:ARG:HB2	2.48	0.43
1:C:659:ASN:OD1	1:C:660:GLY:N	2.52	0.43
1:D:593:GLU:OE1	1:D:593:GLU:HA	2.18	0.42
1:D:614:LEU:HD23	1:D:614:LEU:HA	1.86	0.42
1:E:565:SER:OG	1:E:633:GLU:HG3	2.19	0.42
1:A:684:TRP:CE3	1:A:737:TRP:HA	2.55	0.42
1:B:597:SER:O	1:B:601:VAL:HG23	2.20	0.42
1:E:471:TRP:CD1	1:E:536:LYS:HE2	2.55	0.42
1:A:694:PHE:CZ	1:A:729:LEU:HD13	2.54	0.41
1:B:699:SER:HA	1:B:700:PRO:HD3	1.83	0.41
1:D:581:LEU:O	1:D:582:GLU:HB2	2.18	0.41
1:D:684:TRP:CE3	1:D:737:TRP:HA	2.55	0.41
1:B:518:SER:O	6:B:2017:HOH:O	2.22	0.41
1:B:632:THR:HG21	1:B:638:LYS:HE2	2.02	0.41
1:D:594:GLN:HB2	1:D:595:LEU:H	1.71	0.41
1:D:471:TRP:CD1	1:D:536:LYS:HE2	2.56	0.41
1:B:762:SER:C	1:B:764:GLN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:705:PRO:O	6:E:2014:HOH:O	2.22	0.41
1:E:730:TYR:O	1:E:734:ARG:HG2	2.20	0.41
1:A:576:ARG:HG2	1:A:592:GLU:HB3	2.03	0.41
1:C:471:TRP:CD1	1:C:536:LYS:HE2	2.55	0.41
1:C:659:ASN:HD21	1:D:522:GLU:CD	2.23	0.41
1:C:522:GLU:HG3	6:C:2015:HOH:O	2.21	0.40
1:C:647:ASP:OD1	1:C:649:HIS:ND1	2.37	0.40
1:E:694:PHE:CZ	1:E:729:LEU:HD13	2.55	0.40
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.83	0.40
1:E:598:LYS:HD3	1:E:761:THR:OG1	2.21	0.40
1:E:504:LYS:CE	1:E:507:ARG:NH2	2.84	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	292/310 (94%)	275 (94%)	17 (6%)	0	100	100
1	B	292/310 (94%)	280 (96%)	12 (4%)	0	100	100
1	C	279/310 (90%)	265 (95%)	14 (5%)	0	100	100
1	D	287/310 (93%)	277 (96%)	10 (4%)	0	100	100
1	E	248/310 (80%)	223 (90%)	24 (10%)	1 (0%)	30	49
All	All	1398/1550 (90%)	1320 (94%)	77 (6%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	705	PRO

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	258/270 (96%)	254 (98%)	4 (2%)	55	77
1	B	259/270 (96%)	254 (98%)	5 (2%)	50	73
1	C	248/270 (92%)	242 (98%)	6 (2%)	43	68
1	D	253/270 (94%)	251 (99%)	2 (1%)	73	87
1	E	223/270 (83%)	214 (96%)	9 (4%)	28	52
All	All	1241/1350 (92%)	1215 (98%)	26 (2%)	48	71

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	SER
1	A	462	GLU
1	A	482	LYS
1	A	592	GLU
1	B	460	VAL
1	B	545	ILE
1	B	619[A]	CYS
1	B	619[B]	CYS
1	B	656	LYS
1	C	493	VAL
1	C	498	ILE
1	C	507	ARG
1	C	537	MET
1	C	633	GLU
1	C	708	GLU
1	D	592	GLU
1	D	689	LEU
1	E	492	VAL
1	E	506	ASN
1	E	508	VAL
1	E	516	LEU
1	E	540	LYS
1	E	570	ARG

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Mol	Chain	Res	Type
1	E	664	VAL
1	E	714	LYS
1	E	724	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	743	GLN
1	B	543	ASN
1	B	680	GLN
1	B	727	ASN
1	C	553	GLN
1	D	543	ASN
1	D	659	ASN
1	D	727	ASN
1	E	543	ASN
1	E	680	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](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 for Mogul analysis.

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	SO4	B	1765	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	D	1768	-	4,4,4	0.33	0	6,6,6	0.40	0
2	SO4	E	1762	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	D	1767	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	1765	-	4,4,4	0.24	0	6,6,6	0.07	0
5	PGE	D	1769	-	9,9,9	0.31	0	8,8,8	0.32	0
3	ACT	A	1764	-	3,3,3	0.82	0	3,3,3	1.34	0
2	SO4	D	1764	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	C	1764	-	4,4,4	0.23	0	6,6,6	0.08	0
5	PGE	D	1770	-	9,9,9	0.32	0	8,8,8	0.27	0
2	SO4	A	1763	-	4,4,4	0.24	0	6,6,6	0.07	0
5	PGE	D	1771	-	9,9,9	0.31	0	8,8,8	0.32	0
5	PGE	C	1765	-	9,9,9	0.33	0	8,8,8	0.31	0
2	SO4	D	1766	-	4,4,4	0.24	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	D	1771	-	-	5/7/7/7	-
5	PGE	D	1769	-	-	3/7/7/7	-
5	PGE	C	1765	-	-	3/7/7/7	-
5	PGE	D	1770	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1769	PGE	O2-C3-C4-O3
5	D	1770	PGE	O1-C1-C2-O2
5	C	1765	PGE	O2-C3-C4-O3
5	D	1771	PGE	O1-C1-C2-O2
5	D	1770	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
5	D	1769	PGE	O1-C1-C2-O2
5	C	1765	PGE	C4-C3-O2-C2
5	D	1771	PGE	C6-C5-O3-C4
5	D	1771	PGE	C4-C3-O2-C2
5	D	1771	PGE	O3-C5-C6-O4
5	C	1765	PGE	C3-C4-O3-C5
5	D	1769	PGE	C1-C2-O2-C3
5	D	1771	PGE	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1770	PGE	2	0
5	C	1765	PGE	5	0

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	296/310 (95%)	0.32	21 (7%) 22 18	27, 49, 97, 118	0
1	B	292/310 (94%)	0.11	14 (4%) 35 31	18, 39, 85, 106	4 (1%)
1	C	283/310 (91%)	0.29	17 (6%) 27 23	25, 45, 81, 108	2 (0%)
1	D	290/310 (93%)	0.09	18 (6%) 26 22	23, 40, 80, 113	1 (0%)
1	E	258/310 (83%)	1.19	65 (25%) 1 1	33, 71, 108, 120	0
All	All	1419/1550 (91%)	0.38	135 (9%) 14 11	18, 46, 96, 120	7 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	659	ASN	6.7
1	B	460	VAL	5.9
1	C	505	PRO	5.1
1	E	466	PRO	4.6
1	E	520	ALA	4.0
1	E	645	ALA	4.0
1	D	592	GLU	4.0
1	A	579	PRO	4.0
1	E	717	HIS	3.9
1	E	709	LEU	3.9
1	E	702	PRO	3.9
1	E	484	LEU	3.8
1	D	582	GLU	3.8
1	A	584	SER	3.8
1	E	664	VAL	3.6
1	D	581	LEU	3.6
1	E	662	LEU	3.6
1	E	673	PHE	3.6
1	E	704	VAL	3.6
1	E	557	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	716	GLY	3.5
1	B	461	SER	3.5
1	E	711	LYS	3.5
1	C	658	THR	3.4
1	A	580	GLY	3.4
1	B	489	PHE	3.4
1	C	657	THR	3.4
1	A	461	SER	3.3
1	E	570	ARG	3.3
1	C	762	SER	3.3
1	B	488	ALA	3.3
1	E	516	LEU	3.3
1	D	580	GLY	3.2
1	E	701	TYR	3.2
1	C	708	GLU	3.1
1	D	593	GLU	3.1
1	D	708	GLU	3.1
1	E	559	VAL	3.1
1	E	660	GLY	3.1
1	E	710	PHE	3.1
1	A	762	SER	3.1
1	E	521	THR	3.0
1	C	578	PRO	3.0
1	E	491	GLN	3.0
1	E	724	ASN	3.0
1	E	594	GLN	3.0
1	B	579	PRO	3.0
1	E	720	ASP	3.0
1	A	659	ASN	2.8
1	E	761	THR	2.8
1	D	504	LYS	2.8
1	A	462	GLU	2.8
1	A	657	THR	2.8
1	B	487	GLY	2.8
1	E	505	PRO	2.8
1	E	507	ARG	2.8
1	E	695	THR	2.7
1	E	483	PRO	2.7
1	E	663	PRO	2.7
1	A	489	PHE	2.7
1	E	499	GLY	2.7
1	E	493	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	463	TYR	2.7
1	B	464	GLU	2.7
1	D	518	SER	2.7
1	E	672	LEU	2.7
1	D	594	GLN	2.7
1	C	660	GLY	2.6
1	E	703	GLY	2.6
1	B	651	ILE	2.6
1	B	486	GLU	2.6
1	B	463	TYR	2.6
1	D	650	HIS	2.6
1	E	714	LYS	2.6
1	D	484	LEU	2.6
1	E	490	GLY	2.5
1	D	762	SER	2.5
1	E	482	LYS	2.5
1	D	502	LYS	2.5
1	A	583	TYR	2.5
1	D	658	THR	2.5
1	E	525	LEU	2.5
1	E	595	LEU	2.5
1	E	492	VAL	2.5
1	E	705	PRO	2.4
1	E	676	ILE	2.4
1	A	658	THR	2.4
1	A	488	ALA	2.4
1	A	578	PRO	2.4
1	C	592	GLU	2.4
1	E	517	LYS	2.4
1	D	482	LYS	2.4
1	D	485	GLY	2.3
1	C	760	LEU	2.3
1	E	522	GLU	2.3
1	B	658	THR	2.3
1	B	462	GLU	2.3
1	C	763	ASN	2.3
1	E	469	PRO	2.3
1	E	577	ARG	2.3
1	A	485	GLY	2.3
1	E	558	TYR	2.3
1	A	594	GLN	2.2
1	C	465	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	500	LEU	2.2
1	E	696	LEU	2.2
1	A	482	LYS	2.2
1	C	575	ALA	2.2
1	E	551	CYS	2.2
1	E	480	LEU	2.2
1	E	661	ARG	2.2
1	C	500	LEU	2.2
1	E	712	LEU	2.2
1	C	476	ASP	2.2
1	A	483	PRO	2.2
1	E	502	LYS	2.2
1	E	515	MET	2.1
1	E	550	ALA	2.1
1	C	761	THR	2.1
1	E	603	CYS	2.1
1	E	524	ASP	2.1
1	E	574	GLN	2.1
1	B	593	GLU	2.1
1	C	506	ASN	2.1
1	E	677	TYR	2.1
1	E	575	ALA	2.1
1	B	518	SER	2.1
1	E	556	PRO	2.1
1	A	504	LYS	2.0
1	A	460	VAL	2.0
1	D	506	ASN	2.0
1	D	763	ASN	2.0
1	E	691	TRP	2.0
1	E	501	ASP	2.0
1	A	597	SER	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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
4	CL	D	1773	1/1	0.53	0.41	96,96,96,96	0
2	SO4	D	1767	5/5	0.57	0.15	87,91,116,127	0
3	ACT	A	1764	4/4	0.70	0.17	56,69,70,77	0
4	CL	C	1766	1/1	0.72	0.15	88,88,88,88	0
2	SO4	D	1765	5/5	0.72	0.10	106,108,138,139	0
2	SO4	D	1768	5/5	0.77	0.11	104,112,115,137	0
5	PGE	D	1770	10/10	0.79	0.22	34,73,81,84	0
5	PGE	D	1771	10/10	0.82	0.17	56,74,79,80	0
5	PGE	C	1765	10/10	0.83	0.18	42,54,59,61	0
2	SO4	B	1765	5/5	0.86	0.12	71,93,109,116	0
2	SO4	A	1763	5/5	0.87	0.13	67,76,109,115	0
5	PGE	D	1769	10/10	0.90	0.14	48,66,79,81	0
2	SO4	D	1766	5/5	0.93	0.10	62,65,87,89	0
2	SO4	E	1762	5/5	0.94	0.10	55,56,62,69	0
2	SO4	C	1764	5/5	0.96	0.08	57,66,73,82	0
4	CL	D	1774	1/1	0.97	0.07	38,38,38,38	0
2	SO4	D	1764	5/5	0.98	0.07	35,37,53,64	0
4	CL	D	1772	1/1	0.98	0.07	43,43,43,43	0
4	CL	B	1766	1/1	0.99	0.05	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.