



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:58 AM UTC

PDB ID : 4CCF / pdb_00004ccf
Title : Structure of Respiratory Syncytial Virus F protein head domain
Authors : Peat, T.S.
Deposited on : 2013-10-22
Resolution : 2.65 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)
Xtrriage (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

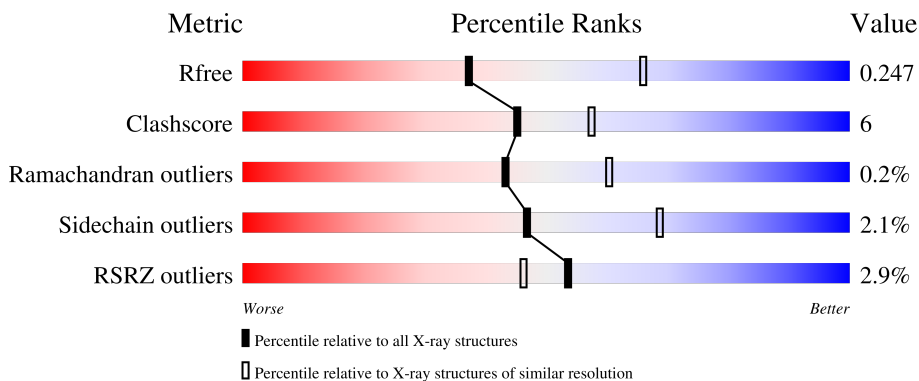
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



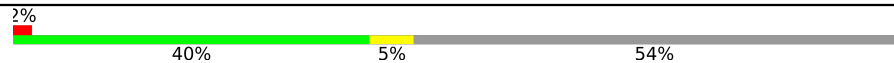
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	574	2% 40% 6% 54%
1	B	574	% 40% 5% 55%
1	C	574	2% 40% 5% 55%
1	D	574	% 40% 7% 53%
1	E	574	% 39% 5% 55%

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Mol	Chain	Length	Quality of chain
1	F	574	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a green segment labeled '40%', a yellow segment labeled '5%', and a large grey segment at the end labeled '54%'.</p>

2 Entry composition [i](#)

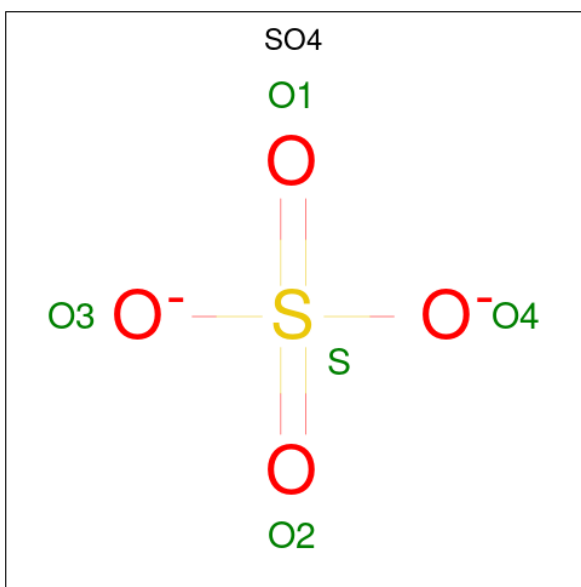
There are 3 unique types of molecules in this entry. The entry contains 12234 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FUSION GLYCOPROTEIN F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	Total 2036	C 1278	N 338	O 402	S 18	0	0	0
1	B	258	Total 1995	C 1251	N 331	O 395	S 18	0	0	0
1	C	261	Total 2026	C 1272	N 335	O 401	S 18	0	1	0
1	D	268	Total 2080	C 1309	N 343	O 410	S 18	0	1	0
1	E	257	Total 2005	C 1258	N 333	O 396	S 18	0	2	0
1	F	265	Total 2041	C 1281	N 338	O 404	S 18	0	1	0

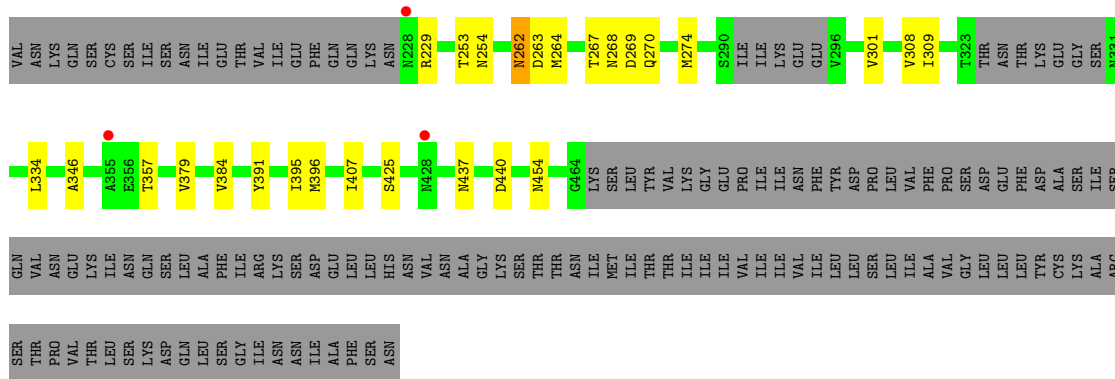
- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



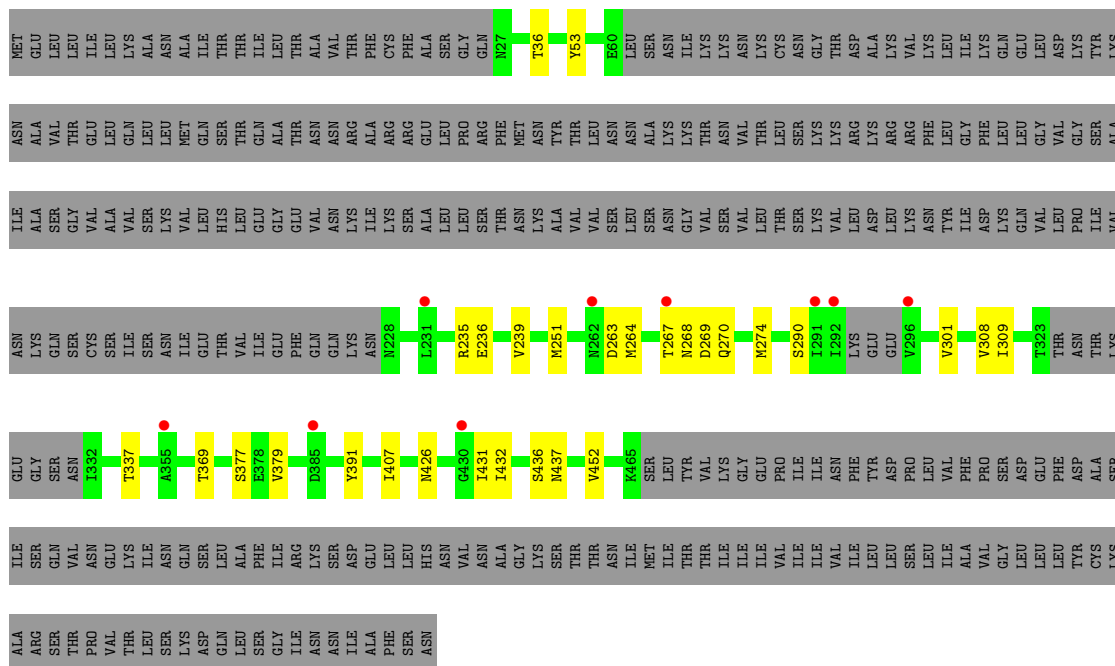
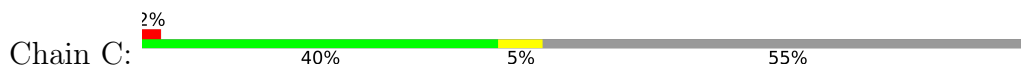
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

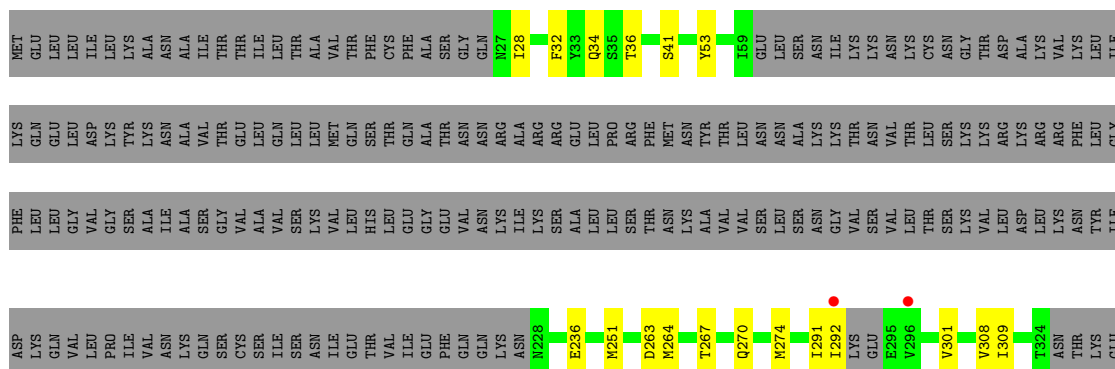
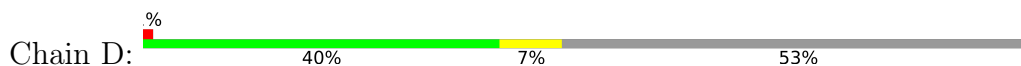
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	6	Total	O	0	0
			6	6		
3	C	6	Total	O	0	0
			6	6		
3	D	3	Total	O	0	0
			3	3		
3	E	8	Total	O	0	0
			8	8		
3	F	5	Total	O	0	0
			5	5		



● Molecule 1: FUSION GLYCOPROTEIN F0



● Molecule 1: FUSION GLYCOPROTEIN F0



ASN
GLU
LYS
ILE
ASN
GLN
SER
LEU
ALA
PHE
ILE
ARG
LYS
SER
SER
ASP
GLU
LEU
LEU
HIS
ASN
VAL
VAL
ASN
ALA
GLY
LYS
SER
THR
THR
ASN
ILE
MET
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THR
THR
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SER
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GLY
LEU
LEU
TYR
CYS
LYS
ALA
ARG
SER
THR

PRO
VAL
THR
SER
LYS
ASP
GLN
LEU
SER
GLY
ILE
ASN
ASN
ILE
ALA
PHE
SER
ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.38Å 133.50Å 116.42Å 90.00° 93.32° 90.00°	Depositor
Resolution (Å)	43.07 – 2.65 43.07 – 2.65	Depositor EDS
% Data completeness (in resolution range)	87.7 (43.07-2.65) 87.8 (43.07-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.215 , 0.247 0.215 , 0.247	Depositor DCC
R_{free} test set	2763 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12234	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

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	0.80	0/2068	0.96	1/2811 (0.0%)
1	B	0.78	0/2026	0.92	2/2751 (0.1%)
1	C	0.79	0/2057	0.93	1/2793 (0.0%)
1	D	0.76	0/2112	0.95	2/2868 (0.1%)
1	E	0.78	0/2036	0.91	1/2764 (0.0%)
1	F	0.79	0/2073	0.95	3/2817 (0.1%)
All	All	0.78	0/12372	0.94	10/16804 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	428	ASN	N-CA-C	-7.37	100.81	110.53
1	F	432	ILE	CB-CA-C	-7.29	102.76	111.94
1	A	364	ARG	CB-CG-CD	-6.42	96.52	111.30
1	D	333	CYS	N-CA-CB	-5.65	100.90	111.13
1	F	264	MET	CG-SD-CE	5.38	112.73	100.90
1	B	425	SER	N-CA-C	5.27	117.69	109.52
1	D	425	SER	N-CA-C	5.15	117.50	109.52
1	C	377	SER	N-CA-C	5.13	117.61	111.71
1	B	357	THR	N-CA-C	5.11	117.59	111.71
1	E	425	SER	N-CA-C	5.08	117.39	109.52

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	2036	0	2005	28	1
1	B	1995	0	1972	17	0
1	C	2026	0	2003	17	0
1	D	2080	0	2061	36	0
1	E	2005	0	1986	27	1
1	F	2041	0	2005	32	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
3	A	8	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	3	0	0	0	0
3	E	8	0	0	0	0
3	F	5	0	0	0	0
All	All	12234	0	12032	144	1

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 6.

All (144) 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:334:LEU:HB3	1:B:395:ILE:HD11	1.07	1.03
1:A:385:ASP:O	1:A:388:ASN:ND2	1.93	1.01
1:A:311:THR:HG21	1:A:344:ASP:O	1.65	0.96
1:E:311:THR:HG21	1:E:344:ASP:O	1.68	0.94
1:B:270:GLN:HG2	1:B:309:ILE:HD12	1.53	0.90
1:B:334:LEU:HB3	1:B:395:ILE:CD1	2.01	0.87
1:D:388:ASN:C	1:D:388:ASN:HD22	1.87	0.82
1:F:58:THR:CG2	1:F:296:VAL:HG21	2.10	0.81
1:D:36:THR:CG2	1:D:336:ARG:HD2	2.13	0.79
1:F:270:GLN:HG2	1:F:309[A]:ILE:HD12	1.65	0.77
1:A:270:GLN:HG2	1:A:309:ILE:HD12	1.66	0.77
1:D:270:GLN:HG2	1:D:309[A]:ILE:HD12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:GLN:HG2	1:C:309:ILE:HD12	1.67	0.75
1:D:389:PRO:O	1:E:399:LYS:NZ	2.20	0.70
1:D:36:THR:HG22	1:D:336:ARG:HD2	1.73	0.70
1:D:402:VAL:HG13	1:F:374:THR:HG22	1.76	0.67
1:B:334:LEU:CB	1:B:395:ILE:HD11	2.03	0.67
1:D:465:LYS:O	1:F:55:SER:OG	2.12	0.67
1:C:36:THR:O	3:C:2001:HOH:O	2.11	0.66
1:D:388:ASN:O	1:D:388:ASN:ND2	2.27	0.66
1:C:264:MET:HE1	1:C:274:MET:SD	2.37	0.65
1:B:229:ARG:NH2	1:B:253:THR:OG1	2.31	0.64
1:A:264:MET:HE1	1:A:274:MET:SD	2.38	0.63
1:E:264:MET:HE1	1:E:274:MET:SD	2.38	0.63
1:B:264:MET:HE1	1:B:274:MET:SD	2.38	0.63
1:D:264:MET:HE1	1:D:274:MET:SD	2.38	0.63
1:D:291:ILE:HG22	1:D:292:ILE:N	2.14	0.62
1:A:386:ILE:HD11	1:A:395:ILE:HG21	1.81	0.61
1:D:36:THR:OG1	1:D:383:ASN:O	2.12	0.60
1:A:58:THR:HG23	1:A:296:VAL:CG1	2.31	0.60
1:F:436:SER:OG	1:F:437:ASN:N	2.35	0.59
1:C:426:ASN:HB2	1:C:432:ILE:HD11	1.82	0.59
1:A:426:ASN:HB2	1:A:432:ILE:HD11	1.85	0.58
1:C:436:SER:OG	1:C:437:ASN:N	2.32	0.58
1:F:270:GLN:HG2	1:F:309[B]:ILE:HD13	1.85	0.58
1:F:58:THR:HG23	1:F:296:VAL:HG21	1.86	0.58
1:F:264:MET:HE2	1:F:303:LEU:HD12	1.85	0.57
1:D:388:ASN:ND2	1:D:391:TYR:O	2.33	0.57
1:D:354:GLN:NE2	1:E:354:GLN:OE1	2.38	0.56
1:E:388[A]:ASN:C	1:E:388[A]:ASN:HD22	2.13	0.56
1:E:388[A]:ASN:ND2	1:E:391:TYR:O	2.38	0.56
1:F:31:GLU:HG2	1:F:33:TYR:CZ	2.41	0.55
1:F:58:THR:CG2	1:F:296:VAL:CG2	2.84	0.55
1:A:423:THR:HG22	1:A:424:ALA:N	2.22	0.54
1:A:58:THR:HG23	1:A:296:VAL:HG13	1.90	0.54
1:B:270:GLN:HG2	1:B:309:ILE:CD1	2.31	0.54
1:E:401:ASP:OD2	1:E:418:GLY:N	2.41	0.54
1:A:253:THR:HG22	1:A:254:ASN:N	2.23	0.53
1:D:291:ILE:HG22	1:D:292:ILE:H	1.75	0.53
1:E:47:ALA:HA	1:E:309[A]:ILE:HD13	1.91	0.52
1:E:346:ALA:CB	1:F:452:VAL:HG12	2.39	0.52
1:D:36:THR:HG22	1:D:336:ARG:CD	2.40	0.52
1:D:334:LEU:HD11	1:D:386:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ILE:HG23	1:A:387:PHE:CD2	2.46	0.51
1:D:334:LEU:CD1	1:D:386:ILE:HD13	2.41	0.51
1:E:46:SER:OG	1:E:311:THR:HB	2.11	0.51
1:E:388[A]:ASN:ND2	1:E:388[A]:ASN:O	2.42	0.51
1:D:32:PHE:CE2	1:D:34:GLN:HG2	2.47	0.50
1:F:270:GLN:HG2	1:F:309[B]:ILE:CD1	2.41	0.50
1:B:253:THR:HG22	1:B:254:ASN:N	2.26	0.50
1:E:267:THR:HG22	1:E:268:ASN:N	2.27	0.50
1:A:386:ILE:HD11	1:A:395:ILE:CG2	2.42	0.50
1:D:334:LEU:HB2	1:D:395:ILE:HG21	1.94	0.49
1:F:267:THR:HG22	1:F:268:ASN:N	2.28	0.49
1:A:46:SER:OG	1:A:311:THR:HB	2.11	0.49
1:F:426:ASN:HB2	1:F:432:ILE:HD11	1.94	0.49
1:D:267:THR:OG1	1:D:270:GLN:HG3	2.12	0.49
1:F:428:ASN:O	1:F:429:ARG:HB2	2.12	0.49
1:E:311:THR:HG23	1:E:344:ASP:HB2	1.94	0.49
1:A:58:THR:HG23	1:A:296:VAL:HG11	1.95	0.49
1:D:28:ILE:HD11	1:D:363:ASN:CB	2.42	0.49
1:A:270:GLN:HG2	1:A:309:ILE:CD1	2.40	0.49
1:D:388:ASN:C	1:D:388:ASN:ND2	2.57	0.49
1:F:270:GLN:HG2	1:F:309[A]:ILE:CD1	2.40	0.48
1:B:267:THR:HG22	1:B:268:ASN:N	2.28	0.48
1:A:311:THR:HG23	1:A:344:ASP:HB2	1.95	0.48
1:C:270:GLN:HG2	1:C:309:ILE:CD1	2.41	0.48
1:E:53:TYR:CZ	1:F:464:GLY:HA3	2.49	0.48
1:D:466:SER:O	1:D:467:LEU:HD23	2.14	0.48
1:F:58:THR:HG23	1:F:296:VAL:CG2	2.44	0.47
1:F:427:LYS:HG2	1:F:448:ASP:OD2	2.15	0.47
1:E:442:VAL:CG1	1:E:447:VAL:HG21	2.45	0.47
1:C:267:THR:HG22	1:C:268:ASN:N	2.29	0.46
1:E:442:VAL:HG13	1:E:447:VAL:HG21	1.97	0.46
1:F:58:THR:HG22	1:F:296:VAL:HG21	1.94	0.46
1:E:388[B]:ASN:OD1	1:E:389:PRO:HD2	2.16	0.46
1:D:270:GLN:HG2	1:D:309[A]:ILE:CD1	2.41	0.46
1:A:267:THR:OG1	1:A:270:GLN:HG3	2.15	0.46
1:A:423:THR:HG23	1:A:433:LYS:O	2.15	0.46
1:D:397:THR:HG22	1:D:398:SER:N	2.30	0.46
1:E:53:TYR:OH	1:E:263:ASP:OD2	2.34	0.46
1:D:291:ILE:CG2	1:D:292:ILE:N	2.78	0.46
1:B:308:VAL:C	1:B:309:ILE:HG13	2.40	0.45
1:A:53:TYR:OH	1:A:263:ASP:OD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:THR:O	1:E:339:ARG:NH2	2.50	0.45
1:C:369:THR:HG22	1:C:369:THR:O	2.16	0.45
1:D:28:ILE:HD11	1:D:363:ASN:HB3	1.98	0.45
1:A:423:THR:CG2	1:A:424:ALA:N	2.80	0.45
1:D:402:VAL:HG13	1:F:374:THR:CG2	2.47	0.45
1:E:401:ASP:C	1:E:401:ASP:OD1	2.59	0.45
1:F:53:TYR:OH	1:F:263:ASP:OD2	2.35	0.44
1:D:291:ILE:CG2	1:D:292:ILE:H	2.31	0.44
1:B:395:ILE:CG1	1:B:396:MET:N	2.81	0.44
1:C:267:THR:HG22	1:C:269:ASP:H	1.83	0.44
1:B:267:THR:HG22	1:B:269:ASP:H	1.82	0.43
1:D:53:TYR:OH	1:D:263:ASP:OD2	2.34	0.43
1:A:236:GLU:OE2	1:C:239:VAL:HG22	2.18	0.43
1:E:267:THR:HG22	1:E:269:ASP:H	1.83	0.43
1:E:388[A]:ASN:C	1:E:388[A]:ASN:ND2	2.76	0.43
1:F:267:THR:HG22	1:F:269:ASP:H	1.83	0.43
1:A:308:VAL:C	1:A:309:ILE:HG13	2.44	0.43
1:B:53:TYR:OH	1:B:263:ASP:OD2	2.35	0.43
1:B:346:ALA:CB	1:C:452:VAL:HG12	2.49	0.43
1:D:395:ILE:HG22	1:D:396:MET:N	2.33	0.43
1:A:388:ASN:ND2	1:A:388:ASN:H	2.17	0.43
1:C:53:TYR:OH	1:C:263:ASP:OD2	2.35	0.43
1:B:379:VAL:HG12	1:B:391:TYR:CE2	2.54	0.43
1:E:401:ASP:OD2	1:E:417:TYR:C	2.62	0.43
1:F:427:LYS:HG3	1:F:428:ASN:H	1.83	0.42
1:A:236:GLU:OE1	1:A:251:MET:HE2	2.19	0.42
1:F:426:ASN:HB3	1:F:428:ASN:O	2.19	0.42
1:C:337:THR:HG22	1:C:337:THR:O	2.18	0.42
1:C:236:GLU:OE1	1:C:251:MET:HE2	2.19	0.42
1:C:308:VAL:C	1:C:309:ILE:HG13	2.45	0.42
1:F:337:THR:O	1:F:337:THR:HG22	2.19	0.42
1:F:429:ARG:HB3	1:F:430:GLY:H	1.68	0.42
1:A:264:MET:HE1	1:A:274:MET:HE1	2.01	0.41
1:B:308:VAL:O	1:B:309:ILE:HG13	2.20	0.41
1:D:379:VAL:HG12	1:D:391:TYR:CE2	2.55	0.41
1:A:232:GLU:OE2	1:C:235:ARG:NH1	2.53	0.41
1:B:262:ASN:OD1	1:D:466:SER:HB2	2.21	0.41
1:D:402:VAL:CG1	1:F:374:THR:HG22	2.47	0.41
1:E:236:GLU:OE1	1:E:251:MET:HE2	2.20	0.41
1:D:236:GLU:OE1	1:D:251:MET:HE2	2.20	0.41
1:D:308:VAL:C	1:D:309[A]:ILE:HG13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:THR:HA	1:A:246:PRO:C	2.45	0.41
1:F:245:THR:HA	1:F:246:PRO:C	2.46	0.40
1:A:364:ARG:HD3	1:A:364:ARG:HA	1.78	0.40
1:E:401:ASP:OD1	1:E:402:VAL:N	2.54	0.40
1:E:53:TYR:OH	1:F:464:GLY:HA3	2.21	0.40
1:F:464:GLY:O	1:F:465:LYS:C	2.64	0.40
1:C:379:VAL:HG12	1:C:391:TYR:CE2	2.56	0.40
1:E:309[B]:ILE:HG12	1:E:310:ASP:N	2.37	0.40
1:F:429:ARG:NH1	1:F:432:ILE:HG23	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASP:OD2	1:E:42:LYS:NZ[1_656]	2.10	0.10

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	259/574 (45%)	248 (96%)	11 (4%)	0	100 100
1	B	250/574 (44%)	242 (97%)	7 (3%)	1 (0%)	30 45
1	C	254/574 (44%)	247 (97%)	7 (3%)	0	100 100
1	D	261/574 (46%)	250 (96%)	10 (4%)	1 (0%)	30 45
1	E	251/574 (44%)	245 (98%)	5 (2%)	1 (0%)	30 45
1	F	260/574 (45%)	248 (95%)	12 (5%)	0	100 100
All	All	1535/3444 (45%)	1480 (96%)	52 (3%)	3 (0%)	43 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	437	ASN
1	B	437	ASN
1	E	437	ASN

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	239/520 (46%)	233 (98%)	6 (2%)	42	64
1	B	237/520 (46%)	231 (98%)	6 (2%)	42	64
1	C	240/520 (46%)	236 (98%)	4 (2%)	53	73
1	D	246/520 (47%)	241 (98%)	5 (2%)	48	69
1	E	238/520 (46%)	233 (98%)	5 (2%)	47	69
1	F	239/520 (46%)	234 (98%)	5 (2%)	47	69
All	All	1439/3120 (46%)	1408 (98%)	31 (2%)	47	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	LEU
1	A	292	ILE
1	A	301	VAL
1	A	311	THR
1	A	357	THR
1	A	407	ILE
1	B	262	ASN
1	B	301	VAL
1	B	384	VAL
1	B	407	ILE
1	B	440	ASP
1	B	454	ASN
1	C	290	SER
1	C	301	VAL
1	C	407	ILE
1	C	431	ILE

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Mol	Chain	Res	Type
1	D	41	SER
1	D	301	VAL
1	D	388	ASN
1	D	395	ILE
1	D	407	ILE
1	E	301	VAL
1	E	311	THR
1	E	354	GLN
1	E	388[A]	ASN
1	E	388[B]	ASN
1	F	291	ILE
1	F	301	VAL
1	F	357	THR
1	F	407	ILE
1	F	432	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	ASN
1	B	27	ASN
1	B	34	GLN
1	B	268	ASN
1	B	454	ASN
1	C	34	GLN
1	D	380	ASN
1	E	34	GLN
1	E	380	ASN
1	F	34	GLN
1	F	268	ASN
1	F	426	ASN

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](#)

3 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	SO4	E	1466	-	4,4,4	0.49	0	6,6,6	0.43	0
2	SO4	C	1466	-	4,4,4	0.35	0	6,6,6	1.04	0
2	SO4	D	1470	-	4,4,4	0.54	0	6,6,6	0.23	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	265/574 (46%)	0.13	13 (4%) 35 27	18, 38, 65, 107	1 (0%)
1	B	258/574 (44%)	0.09	5 (1%) 66 61	17, 37, 70, 91	0
1	C	261/574 (45%)	0.02	9 (3%) 48 40	16, 34, 64, 92	1 (0%)
1	D	268/574 (46%)	0.05	5 (1%) 66 61	19, 40, 66, 85	1 (0%)
1	E	257/574 (44%)	0.05	4 (1%) 70 66	13, 37, 65, 107	2 (0%)
1	F	265/574 (46%)	0.05	9 (3%) 48 40	15, 36, 69, 97	1 (0%)
All	All	1574/3444 (45%)	0.07	45 (2%) 53 46	13, 37, 68, 107	6 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	4.9
1	C	355	ALA	4.8
1	D	355	ALA	4.6
1	D	296	VAL	3.9
1	C	296	VAL	3.5
1	B	355	ALA	3.4
1	C	291	ILE	3.2
1	A	60	GLU	3.0
1	B	57	ILE	3.0
1	A	295	GLU	2.9
1	A	292	ILE	2.9
1	A	436	SER	2.8
1	C	292	ILE	2.7
1	C	262	ASN	2.6
1	E	355	ALA	2.5
1	F	228	ASN	2.5
1	F	263	ASP	2.5
1	A	293	LYS	2.3
1	C	430	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	231	LEU	2.3
1	F	231	LEU	2.3
1	A	323	THR	2.2
1	E	434	THR	2.2
1	F	354	GLN	2.2
1	D	469	VAL	2.2
1	E	332	ILE	2.2
1	F	332	ILE	2.2
1	C	267	THR	2.2
1	B	428	ASN	2.2
1	C	231	LEU	2.2
1	A	296	VAL	2.2
1	F	428	ASN	2.2
1	D	361	GLN	2.2
1	A	263	ASP	2.2
1	A	291	ILE	2.2
1	F	60	GLU	2.1
1	B	59	ILE	2.1
1	C	385	ASP	2.1
1	F	431	ILE	2.1
1	F	355	ALA	2.1
1	B	228	ASN	2.1
1	D	292	ILE	2.1
1	A	259	SER	2.0
1	A	59	ILE	2.0
1	E	59	ILE	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 oligosaccharides 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(\AA^2)	Q<0.9
2	SO4	D	1470	5/5	0.94	0.07	57,59,64,69	0
2	SO4	E	1466	5/5	0.96	0.09	53,56,58,64	0
2	SO4	C	1466	5/5	0.99	0.05	26,26,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.